SIAM 2021 Summer Conferences

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SIAM Annual Meeting (AN21)

July 19 – 23, 2021

SIAM Conference on Applied & Computational Discrete Algorithms (ACDA21)

July 19 – 21, 2021

SIAM Conference on Control and Its Applications (CT21)

July 19 – 21, 2021

SIAM Conference on Discrete Mathematics (DM21)

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SIAM Conference on Optimization (OP21)

July 20 – 23, 2021

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Annual Meeting

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IP1

Opening Remarks and Presentation: Scientific Uses of Automatic Differentiation

Automatic differentiation packages have enabled and are enabling recent advances in machine learning. But they also have other uses for scientific computation and discovery. I will outline a number of different directions we have been undertaking using automatic differentiation and large scale optimization to solve science problems, including developing new algorithms for solving partial differential equations, the design of energy landscapes and kinetic pathways for self assembly, the discovery of unstable solutions controlling fluid dynamical instabilities, the development of models for organismal development and implementing statistical mechanics algorithms for realistic protein self assembly.

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IP2

Machine Learning for Multi-Scale Systems: From Turbulence to Climate Prediction

Many problems encountered in the sciences, from engineering to climate, involve multi-scale phenomena, such as turbulence. These problems are often intractable computationally due to the high number of degrees of freedom necessary to resolve all the dynamically relevant scales. In this talk, I will discuss how the availability of climate data and machine learning algorithms are helping to overcome the curse of dimensionality and discover hidden physics. I will present some of our recent work combining physics and machine learning to deepen our understanding of turbulent processes and provide more reliable climate simulations. The topics will include using deep learning to learn turbulence models from high-dimensional data, quantifying uncertainties associated with learned representations of turbulence, combining physical conservation laws with machine learning, and discovering closed-form equations of ocean turbulence models from data.

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IP3

Wave Propagation and Correlation-Based Imaging in Random Media

Wave-based imaging in complex media has important applications in medical imaging, nondestructive testing, and seismology for instance. In this talk we consider direct and inverse problems related to wave propagation in complex media. The modeling of complex media by random processes and the use of separation of scales techniques make it possible to study the statistics of the wave field. This study in turn helps in characterizing imaging algorithms that use the signals recorded by receiver arrays and transmitted by controlled or opportunistic sources. The assessment of the stability and resolution properties of these algorithms is challenging. Indeed, the required inputs of the algorithms are typically cross correlations or Wigner transforms, which are expectations with respect to the distribution of the random medium. However, only empirical quantities can be extracted from the recorded signals, which are not in general statistically stable in the sense that their typical values can be different from their expectations. Smoothing of the empirical quantities is then required to get stability, but also leads to a loss of resolution. We will see how to achieve optimal trade-off between stability and resolution and describe situations where correlation-based imaging can be efficient or not.

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IP4

Convergence of AI, Simulations and HPC

Many scientific applications heavily rely on the use of brute-force numerical methods performed on high-performance computing (HPC) infrastructure. Can artificial intelligence (AI) methods augment or even entirely replace these brute-force calculations to obtain significant speed-ups? Can we make groundbreaking new discoveries as a result of such speed-ups? I will present exciting recent advances that build new foundations in AI that are applicable to a wide range of problems such as fluid dynamics and quantum chemistry. On the other side of the coin, the use of simulations to train AI models can be very effective in applications such as robotics and autonomous driving. Thus, we will see a convergence of AI, Simulations and HPC in the coming years.

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IP5

Selective Inference for Trees

As datasets grow in size, the focus of data collection has increasingly shifted away from testing pre-specified hypotheses, and towards hypothesis generation. Researchers are often interested in performing an exploratory data analysis to generate hypotheses, and then testing those hypotheses on the same data. Unfortunately, this type of 'double dipping' can lead to highly-inflated Type 1 errors. In this talk, I will consider double-dipping on trees. First, I will focus on trees generated via hierarchical clustering, and will consider testing the null hypothesis of equality of cluster means. I will propose a test for a difference in means between estimated clusters that accounts for the cluster estimation process, using a selective inference framework. Second, I'll consider trees generated using the CART procedure, and will again use selective inference to conduct inference on the means of the terminal nodes. Applications include single-cell RNA-sequencing data and the Box Lunch Study. This is collaborative work with Lucy Gao (U. Waterloo), Anna Neufeld (U. Washington), and Jacob Bien (USC).

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IP6

Randomized Algorithms for Linear Algebraic Computations

The talk will describe how randomized algorithms can effectively, accurately, and reliably solve linear algebraic problems that are omnipresent in scientific computing and in data analysis. We will focus on techniques for low rank approximation, since these methods are particularly simple and powerful. The talk will also briefly survey a number of other randomized algorithms for tasks such as solving linear systems, estimating matrix norms, and computing full matrix factorizations.

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IP7

Invited Speaker Title TBA - Whitfield

To follow.

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IP8

Closing Remarks and Presentation: Dispersive Hydrodynamics: Dispersive Shock Waves, Solitons, and (Non)Convexity

Dispersive hydrodynamics encapsulate a rich class of multiscale nonlinear wave problems in dispersive media that are epitomized by the dispersive shock wave (DSW), an expanding, highly oscillatory wavetrain between two distinct equilibirum states. Modeled by first order systems of conservation laws modified by higher order conservative terms, DSWs occur in a variety of physical environments ranging from the large (e.g., geophysical fluids) to the small (e.g., optical, matter, and spin waves). This talk will present recent developments toward a general description of DSWs using nonlinear wave modulation theory, an asymptotic description in the small dispersion regime. As an added bonus, solitons or solitary waves and their interactions with dispersive hydrodynamic flows are described by the same equations through an appropriate limit. A key concept to the analysis is the strict hyperbolicity and genuine nonlinearity (convexity) of the modulation equations. For nonconvex systems, a variety of new DSW solutions are shown to arise. Fluid experiments highlighting some of the theoretical findings will also be shared.

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IP9

Invited Speaker Title TBA - Bourouiba

To follow.

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IP10

Sparse Integer Solutions of Systems of Linear Equations

The *sparsity* of a solution of a linear system of equations is the number of its nonzero entries, also called the ℓ_0-norm of the vector. A solution is *sparse* if the sparsity is small. Sparse real solutions of linear systems are relevant for signal processing and they have remarkable structure useful in inverse problems and image processing. For instance, Candes and Tao showed a linear programming relaxation provides a good approximation to the sparsest real solution. In this lecture I will discuss the closely related problem of finding sparse integer solutions of linear systems. My own motivation comes from combinatorial optimization, because severa problems have useful interpretations based on sparse representations of elements in a lattice or a semigroup. For example, the minimum edge-coloring problem of graphs can be seen as a problem in the semigroup generated by the matchings of the input graph I discuss several new and old results about the sparsity ofthe solutions to systems of linear Diophantine equations with and without non-negativity of variables. This is all joint work with Iskander Aliev (Cardiff Univ), Gennadiy Averkov (BTU Cottbus - Senftenberg) and Timm Oertel (Cardiff Univ).

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SP1

AWM-SIAM Sonia Kovalevsky Lecture ¡BR¿From Linear Poroelasticity to Nonlinear Implicit Elastic and Related Models

Poroelasticity has many applications in energy and environmental engineering. When linear, it simulates the transient flow of a single-phase fluid in a deformable linear elastic porous medium. However, when the medium is brittle and fractured, linear elasticity is not applicable, but new nonlinear implicit models lead to a good description of the phenomenon. I shall introduce the simplest model of poroelasticity, then describe some new models and explain their mathematical and numerical issues. Collaborators: Tameem Almani, Andrea Bonito, Saumik Dana, Benjamin Ganis, Mara Gonzlez Taboada, Diane Guignard, Frdric Hecht, Kundan Kumar, Xueying Lu, Marc Mear, Kumbakonam Rajagopal, Gurpreet Singh, Endre Sli, Mary Wheeler.

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SP2

I. E. Block Community Lecture¡br¿Can You Hear the Will of the People in the Vote? Assessing Fairness in Redistricting via Monte Carlo Sampling

The US political system chooses representatives to localized geographic districts. Every 10 years, the census counts the population, requiring new districts. Gerrymandering is the harnessing of this administrative process for partisan political gain. The release of the new Census numbers in the Fall of 2021, has again moved redistricting into the national consciousness. Society is confronted with the need to create/evaluate districting maps. Can we recognize gerrymandering when we see it? Is proportionality relevant? What is fair? How does the geopolitical geometry inform these answers? What is the effect of incumbency protection or the Voting Rights Act or more generally the preservation of communities of interest? Since 2013, my group has developed methods using Monte Carlo sampling to reveal the structure of the map between votes and political outcomes under typical districtings. I have testified in Common Cause v. Rucho and Common Cause v. Lewis which resulted in the redrawing of the NC State Legislative and Congressional map for the 2020 elections. This is a story of the interaction between lawyers, mathematicians, and policy advocates; each group pushing the other. The problem of understanding gerrymandering has also prompted the development of several new computational algorithms which come with new mathematical questions. This is a joint work with G. Herschlag and others including high schoolers and undergduates.

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SP3

The John von Neumann Prize Lecture¡br /¿ High Order Numerical Methods for Hyperbolic Equations

Hyperbolic equations are used extensively in applications including fluid dynamics, astrophysics, electro-magnetism, semi-conductor devices, and biological sciences. High order accurate numerical methods are efficient for solving such partial differential equations, however they are difficult to design because solutions may contain discontinuities. In this talk we will survey several types of high order numerical methods for such problems, including weighted essentially non-oscillatory (WENO) finite difference and finite volume methods, discontinuous Galerkin finite element methods, and spectral methods. We will discuss essential ingredients, properties and relative advantages of each method, and provide comparisons among these methods. Recent development and applications of these methods will also be discussed.

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SP4

Past President's Address¡br¿Mixed Precision Numerical Linear Algebra with More Realistic Error Bounds

As computer architectures evolve, and with the exascale computing era approaching, we face two particular challenges in numerical linear algebra. First, modern hardware increasingly offers low precision floating-point arithmetic, often implemented in a block fused multiply-add operation, and we need to exploit it if we are to extract the best performance from these machines. Second, rounding error bounds are typically proportional to (at least) nu, where n is the problem size and u is the unit roundoff. Already, on today's largest problems, $nu \approx 1$ in single precision, so the error bounds do not guarantee any accuracy. I will describe recent progress in addressing these challenges. Iterative refinement in multiple precisions allows linear systems and least squares problems to be solved with the bulk of the computation in low precision, giving a speedup over algorithms carried out entirely in double precision. New summation techniques help to reduce error bounds with little effect on performance. Finally, probabilistic rounding error analysis shows that under suitable assumptions an error bound nu can be replaced by $\sqrt{n}u$ with high probability—and even by u in some cases.

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SP5

W. T. and Idalia Reid Prize Lecture¡br¿Solution Concepts for Optimal Feedback Control of Nonlinear Partial Differential Equations

Optimal feedback controls for nonlinear systems are characterized by the solutions to a Hamilton Jacobi Bellmann (HJB) equation. In the deterministic case, this is a first order hyperbolic equation. Its dimension is that of the state-space of the nonlinear system. Thus, solving the HJB equation is a formidable task. In case the nonlinear system arises as the discretization of partial differential equation one is confronted with a curse of dimensionality. In practice, optimal feedback controls are frequently based on linearization and subsequent treatment by efficient Riccati solvers. This can be effective, but it is a local procedure, and it may fail or lead to erroneous results. In this talk, I first give a brief survey of current solution strategies to partially cope with this challenging problem. Subsequently I describe three approaches in some detail. The first one is based on Newton steps applied to the HJB equation. Combined with tensor calculus this allows to approximately solve HJB equations up to dimension 100. Results are demonstrated for the control of discretized Fokker Planck equations. The second approach is a data driven technique, which approximated the HJB equation and its gradient from an ensemble of open loop solves. The third technique circumvents the direct solution of the HJB equation. Rather a neural network is trained by means of a succinctly chosen ansatz. It is proven that it approximates the optimal feedback gains as the dimension of the network is increased. This work relies on collaborations with B.Azmi, T.Breiten, S.Dolgov, D.Kalise, L.Pfeiffer, and D.Walter.

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JP1

Joint Plenary Speaker with the SIAM Conference on Applied and Computational Discrete Algorithms¡br¿Towards Scalable and Practical Real-Time Computational Epidemiology

Infectious diseases cause more than 10 million deaths a year worldwide. Globalization, urbanization, climate change, and ecological pressures increase the risk and impact of future pandemics. The ongoing COVID-19 pandemic has exemplified many of these issues. The social, economic, and health impact of the COVID-19 pandemic has been immense and will continue to be felt for decades to come. AI, data science, and scalable computation can play a multifaceted role in reorganizing, augmenting and supporting global real-time epidemic science and the rapid translation to practical public health systems. Since February 2020, our group has been providing local, state, and federal authorities continuous modeling and analytics support to contain the COVID-19 pandemic. The talk will give an overview of the state of the art in real-time computational epidemiology. Then using COVID-19 as an exemplar, we will describe how scalable computing, AI and data science can play an important role in advancing real-time epidemic science. Computational challenges , combinatorial problems and directions for future research will be discussed.

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JP2

Joint Plenary Speaker with the SIAM Conference on Control and Its Applications¡br¿Spiking Control Systems

Spikes are the heart beats of neuronal circuits, event-based cameras, and neuromorphic chips. How shall we control such systems? How shall we make them robust to uncertainty? How shall we design artificial spiking systems that will come even close to the efficiency, resilience, and learning capabilities of natural spiking systems? The control theory of spiking systems is in infancy. Neither analog, nor digital, nor hybrid theories properly acknowledge the distinct feature of spiking. This talk will discuss some of the core questions of spiking control and the potential of spiking communication for the future of control and computation.

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JP3

Joint Plenary Speaker with the SIAM Conference on Optimization¡br¿Augmented Lagrangians and Problem Decomposition in Optimization

An important approach to solving large-scale problems in optimization is decomposing them iteratively into subproblems that are easier to handle numerically. This has long been associated with exploiting block-separable structure in the primal variables by way of solving a dual problem derived from convexity. Without such convexity, problem decomposition techniques have lacked an adequate platform for development. Augmented Lagrangians in nonlinear programming have been recognized as creating local convex duality around a locally optimal solution, but in doing so they thwart decomposition by disrupting separability. Now, however, a path to problem decomposition has opened up that can utilize augmented Lagrangian methodology even in territory beyond just nonlinear programming.

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JP4

Joint Plenary Speaker with the SIAM Conference on Discrete Mathematics ¡br¿Stability in Strategic Queueing Systems

Over the last two decades we have developed good understanding how to quantify the impact of strategic user behavior on outcomes in many games (including traffic routing and online auctions), and showed that the resulting bounds extend to repeated games assuming players use a form of no-regret learning to adapt to the environment. Unfortunately, these results do not apply when outcomes in one round effect the game in the future, as is the case in many applications. In this talk, we study this phenomenon in the context of a game modeling queuing systems: routers compete for servers, where packets that do not get served need to be resent, resulting in a system where the number of packets at each round depends on the success of the routers in the previous rounds. In joint work with Jason Gaitonde, we analyze the resulting highly dependent random process. We find that if the capacity of the servers is high enough to allow a centralized and knowledgeable scheduler to get all packets served even with double the packet arrival rate, then despite selfish behavior of the queues, the expected number of packets in the queues will remain bounded throughout time, assuming older packets have priority. Further, if queues are more patient in evaluating their outcomes, maximizing their long-run success rate, stability can be ensured with just 1.58 times extra capacity, strictly better than what is possible assuming the no-regret property.

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CP1

A Space-Time Spectral Method for the Stokes Problem

In this work, we consider the Stokes equations in steady and unsteady states, along with Dirichlet boundary conditions and an initial condition in the latter case. We impose the $\mathbb{P}_N - \mathbb{P}_{N-2}$ spectral Galerkin scheme in space by using a recombined Legendre polynomial basis resulting in exponential convergence in space. For the unsteady state, we implement spectral collocation in time, thus giving exponential convergence in both space and time. The global spectral operator for both schemes is a saddle point matrix. We prove the 2-norm estimates for every block of the two operator matrices. We proceed to show that the condition number for the global spectral operator for the steady-state scheme is $O(N^4)$, where N is the number of spectral modes in each direction. We have preliminary results on the condition number of the unsteady-state scheme. We also exhibit the numerical results of this scheme applied to the unsteady Navier-Stokes problem.

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CP1

Generalized Perron Frobenius Theory and Solvability of the Absolute Value Equation

Let M be an $n \times n$ square matrix. It is well known that the linear complementarity problem (LCP) (M, q) is uniquely solvable for arbitrary $q \in \mathbb{R}^n$ if and only if M is a P-matrix, i.e., if all its principal minors are positive. Mere solvability of (M, q) for arbitrary q is not yet fully characterized. The general LCP is equivalent to the so-called absolute value equation (AVE) $z - A|z| = b$, where $A \in \mathbb{R}^{n\times n}, b, z \in \mathbb{R}^n$, and $|\cdot|$ denotes the componentwise absolute value. Similar to the LCP-situation, unique solvability of the AVE is completely characterized, but (not necessarily unique) solvability is not. The AVE is uniquely solvable if and only if a quantity called the sign-real spectral radius is smaller than one. We define a similar quantity that we call the aligning spectral radius ρ^a and show that the mapping degree of the piecewise linear function $f : \mathbb{R}^n \to \mathbb{R}^n,\ z \mapsto z - A|z|$ is 1 if $\rho^a(A) < 1$. This implies the existence of an odd number of solutions for the corresponding AVE. Under some slight genericity condition on A, we further show that if ρ^a lies in some small neighborhood about 1, the mapping degree of f is 1 if and only if $\rho^a(A) < 1$. If $n \leq 2$, then f is surjective if and only if $\rho^a(A) < 1$. We compare properties of sign-real and aligning spectral radius and derive criteria for both quantities to coincide.

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CP1

Towards Non-Hermitian Linear Solver Convergence Predictions using Neural Networks

Solving large-scale sparse linear systems by iterative methods is among the most frequent problems in the scientific computing, modelling, learning and simulation of various fields of science and engineering. Meanwhile, experts in these specific domains typically lack the training or knowledge required to select and develop efficient, high-performance implementations of linear solvers with optimal parameters for their own problems, since the convergence speed of these methods (especially for the non-Hermitian systems) depends on a vast of parameters and conditions such as the matrixs spectrum or the right hand side. The conventional way to select a good combination of algorithm and parameters for a specific problem is the auto-tuning techniques, which generates automatically a search space of possible algorithms and parameters, and identifies the most desirable ones through heuristic models. However, the proposition of heuristics for linear solvers can be complicated even for limited parameters. Machine learning can be a better option, to discover the hidden relations between input and output, through a training procedure using large known datasets. This talk presents preliminary results on this topic, using a matrix generator and a neural network, which is to predict how hard will be to compute the solution of a system depending on its properties. In future, it could be possible to compute a good prediction of the time or the number of iteration needed by a given solver.

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CP1

On the Approximation of Low-Rank Rightmost Eigenpairs of a Class of Matrix-Valued Linear Operators

The aim of this talk is to present a new numerical method for approximating leading eigenmatrices, that is associated to the rightmost eigenvalue of the linear operator, in a suitable low-rank manifold. We start introducing an appropriate ordinary differential equation, whose solution allows us to approximate the rightmost eigenpair of the linear operator. From the analysis of the behaviour of such ODE on the whole space, we conclude that, under generic assumptions, the solution converges globally to its leading eigenmatrix, when the rightmost eigenvalue is simple and real. In presence of a simple complex conjugate pair of rightmost eigenvalues, the solution exhibit a periodic behaviour. After that, we leave the whole space for projecting the differential equation on a low-rank manifold of prescribed rank. The projected operator is nonlinear and this makes the its analysis more subtle. In particular, when $\mathcal{A}$ is self-adjoint we are able to prove that the associated low-rank ODE converges (at least locally) to its rightmost eigenmatrix in the low-rank manifold, a property which appears to hold also in the more general case. Finally, we propose two explicit numerical methods, the second being an adaptation of the projector splitting integrator proposed recently by Lubich and Oseledets. The numerical experiments show that the method is effective and competitive.

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CP1

Bohemian Matrices: the Symbolic Computation Approach

Symbolic computation is a powerful tool to investigate mathematical objects and processes by using formal and exact algorithms, prune of rounding errors. In this talk we will show how symbolic computation can be used to deduce some interesting properties, and to conjecture others, on Bohemian matrices, those matrices whose entrees come from a finite population. These properties include answering questions about the rank, the determinants, the eigenvalues, of these finite families of matrices. And, using Symbolic computation in this context, allows the use of parameters in a formal way in order to investigate the nature of these parameters when fixing, both, the entry population and the concrete property considered.

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CP1

Parallel Algorithms for Tensor-Train Decomposi-

tion

The tensor-train (TT) decomposition is a process that expresses a tensor in a data-sparse format so significantly reduce storage and computational costs. In this talk, we propose two parallelizable algorithms that compute the TT format from various tensor inputs: (1) *Parallel-TTSVD* for original format, and (2) *TT-Sketching* for streaming data. For each algorithm, we provide theoretical guarantees of accuracy, along with parallelization methods and scaling analysis. For example, strong scaling results on the Hilbert tensor suggest that both algorithms scale well with the tensor's size. Our parallel algorithms allow users to compute TT formats of large tensors efficiently.

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CP2

Adaptive and Non-Adaptive Boundary Control of the Modified Generalized Korteweg-De Vries-Burgers Equation

We study the nonlinear stabilization problem of the Modified-Generalized Korteweg-de Vries-Burgers (MGKdVB) equation:

$$\frac{\partial u}{\partial t}+\gamma_1 u^\alpha \frac{\partial u}{\partial x}-v\frac{\partial^2 u}{\partial x^2}+\mu\frac{\partial^3 u}{\partial x^3}+\gamma_2\frac{\partial^4 u}{\partial x^4}=0, \quad x\in(0,1),\ t>0, \tag{1}$$

where α is a positive integer and all the parameters $\gamma_1,\ v,\ \mu$ and γ_2 are nonzero known positive constants. We consider the nonlinear non-adaptive and adaptive boundary control problems of the MGKdVB equation subject to $u(0,t)=0$; $u_{xx}(0;t)=0$; $u_x(1,t)=w_1(t)$ and $u_{xx}(1,t)=w_2(t)$; where $w_1(t)$ and $w_2(t)$ present the nonlinear boundary control. First, we propose two nonlinear non-adaptive boundary control laws (i.e., when $\gamma_1,\ v,\ \mu$ and γ_2 are known) for the equation above. Furthermore, four nonlinear adaptive boundary control schemes are proposed for the MGKdVB equation when one of the parameters v or γ_1 is unknown, when both v and γ_1 are unknown and when all the parameters are unknown. Using Lyapunov theorem, we investigate the global exponential stability of the solution in $L_2(0,1)$ for each of the proposed controllers. Last but not least, numerical simulations are given to illustrate the efficiency of the developed control schemes.

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CP2

Sensor Optimisation in Seismic Imaging Via Bilevel Learning

As part of the seismic exploration process, waves are emitted from a source into the earth and sensors record the resulting signal. An image of the subsurface can be created in a process known as Full Waveform Inversion (FWI), which minimises the discrepancies between the measured waves and predicted waves modelled by a PDE. A problem of great practical interest, which is not considered in the standard approach to FWI, is the optimal positioning of the sensors in order to obtain the best return from the seismic exploration process. A key question considered in this talk is "given prior information about the likely make-up of the subsurface (in the form of one or more training models), can one optimise the location of the sensors to retrieve the best possible information about the subsurface?" This problem is considered in the framework of bilevel learning, where the upper level is the sensor optimisation problem, and the lower level is the FWI problem. This talk will present a novel mathematical framework for describing the sensor optimisation algorithm, together with an algorithm for computing the gradient of the upper level problem and a complexity analysis in terms of the number of PDE solves. Numerical illustrations of the algorithm, implemented using BFGS, where the PDE being solved is the wave equation in the frequency domain, are presented showing the benefits of sensor optimisation.

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CP2

On The Exact Solutions of 2D Navier-Stockes Equation In the Plane with Hall

2D nonlinear Navier-Stockes equation with the appropriate initial-boundary conditions is considered in a plane with hall. By the methods of Classical Analysis exact solutions vanishing at infinity are obtained.

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CP2

Global Existence of Solutions to Reaction Diffusion Systems with Mass Transport Type Boundary Conditions on An Evolving Domain

Abstract: We consider reaction-diffusion systems where components diffuse inside the domain and react on the surface through mass transport type boundary conditions on an evolving domain. Using Lyapunov functional and duality arguments, we establish the existence of componentwise non-negative global solutions.

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CP2

Predict Stabilisation Parameter for SUPG using deep learning

Singularly Perturbed PDEs has posed critical challenges for the scientific computing community for decades. Conventional techniques produce spurious oscillations in the numerical solution. Generally, stabilization techniques are employed for reducing spurious oscillations. Streamline Upwind/Petrov-Galerkin(SUPG) is one such popular residual-based stabilization technique very frequently used in research for solving SPDEs. In this method, the extra term depends on a user-defined parameter called stabilization parameter. Finding the optimal value of the stabilization parameter is a challenge. In this work, we have considered the prediction of the stabilization parameter for SUPG using deep neural network. Its a semi-supervised network. In this research work, we have focused on convection-diffusion equations and a detailed deep

learning-based function approximation technique for predicting optimal stabilization parameter for SUPG. The feature set consists of equation coefficients, mesh-size and the spatial location of oscillations/interior layers. In this talk, the initial performance of this technique and the challenges observed will be discussed.

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CP2

Nonlinear Stability of Trivial Solution of Reaction-Diffusion-Convection System

In this presentation, we will consider a reaction-diffusion-convection system in the multidimensional setting, with the non-autonomous terms containing spatially localized reaction terms, that is, they decay to zero at some exponential rate as $|x| \to \infty$, but for the nonlinearities as in the combustion model, that is, having a product structure (start with the nonlinearities of the type $ue^{-\frac{1}{\nu}}$). We will use the exponentially weighted function space to analyze the stability of the trivial solution with respect to spatially localized perturbations with a marginal or unstable essential spectrum, and prove the stability of the zero solution by making nonlinear estimates in weighted spaces.

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CP3

Scaling Theory in Axons and Dendrites

Neurons, the fundamental cellular units of the nervous system, have complex branching processes that connect to one another, forming the basis of information processing and communication in animals. There are a range of cell types that can be classified by differences in structure or function. Here, we use mathematical modeling and biophysical theory to establish a correspondence between neuron structure and function. Using framework from previous work on cardiovascular networks, we develop an objective function minimizing electrical signal conduction time delay and power loss due to dissipation, considering factors unique to neurons such as myelination. We use the method of undetermined Lagrange multipliers to calculate theoretical predictions for scaling ratios of axon and dendrite radius and length in successive levels of the branching network. We test theoretical predictions against image reconstruction data on NeuroMorpho.Org, an online database. We observe differences in the scaling ratios observed between dendrites and axons, as well as between dendrites of cell types with different functions. We find that the data for axons and peripheral nervous system neurons correspond to predictions for conduction time minimization, while the data for dendrites correspond to predictions for power minimization. Our model allows us to extract an allometric scaling relationship between conduction time delay and species size, which is supported by experimental data.

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CP3

Formation and Propagation of Excitation Waves in a Model of Electrically Coupled Pacemaker Cells

Modelling of excitation waves in excitable cells (such as neurons and muscle cells) plays a significant role in understanding the generation and control of various diseases associated with tissue disorder. For example, reflected waves have been associated with the onset of cardiac arrhythmias in the heart. In this work, we consider a reaction-diffusion model to investigate the formation and propagation of excitation waves in coupled pacemaker smooth muscle cells. Numerical simulations of our model show that the interaction of neighbouring cells by diffusive coupling can give rise to several distinctive types of waves including travelling pulses, fronts and spatiotemporal chaos.

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CP3

Epidemic Spread on Patch Networks with Community Structure

Predicting the trajectory of disease epidemics and planning mitigation strategies relies on a knowledge of environmental and socioeconomic factors that affect transmission rates on local and global spatial scales. In this presentation we discuss the simulation of epidemic outbreaks on human metapopulation networks with community structure, such as cities within national boundaries, for which infection rates vary both within and between communities. We demonstrate mathematically that the structures and interactions between these communities, setting aside all other considerations such as disease virulence and human decision-making, have a profound effect on the reproduction rate of the disease throughout the entire network. Under the right circumstances, for example, modifying the number of bridges that connect each neighboring community can increase the reproduction rate of the disease by nearly fifty percent. In this presentation we use this mathematical model to describe several scenarios, such as symptomatic versus asymptomatic diseases, spatial heterogeneity in climate and socioeconomic factors that affect vector habitat suitability, and government intervention that varies in time and among communities. In each of these scenarios, we discuss the importance of community network structure, modularity, internal and external clustering and centrality to the reproduction number and prevalence of epidemic outbreaks.

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CP3

A New Model for Rat-Flea Driven Plague Transmission

Rats have long been thought to drive plague epidemics, specifically bubonic plague. However, an alternative theory for plague transmission has been posited by Dean et al. (PNAS 2018 where ectoparasites living on human hosts drive spread. To demonstrate the human-ectoparasite transmission model, they performed a comparison analysis against existing plague models based on alternate modes of transmission (e.g., rat-flea interactions, human to human pneumonic spread). In their analysis, the human-ectoparasite model predominantly results in the best fit to historical data of plague deaths, suggesting human-ectoparasite interaction to be the principle cause for the spread of plague. In our work here, we present a new mathematical model for the spread of the plague based on rat-flea interactions with the human population. We go on to compare our results versus existing models. Our results suggest that rat-flea transmission of the plague is still plausible. These results contrast with the novel hypothesis that prior plague epidemics were due to human-ectoparasites.

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CP3

Bi-Tensor Free Water Model with Positive Definite Diffusion Tensor and Fast Optimization

Diffusion tensor imaging is a widely used imaging methodology to infer the microstructure of brain tissues. When an image voxel contains partial volume of brain tissue with free water, the traditional one tensor model is not appropriate. A bi-tensor free water model has been proposed to correct for the mixing effects. Moreover, recent studies have shown that the free water volume derived from this model could be a biomarker for brain aging and numerous brain disorders such as Parkinson's and Alzheimer's disease. However, fitting this model is ill-posed without additional assumptions. Models by adding spatial constraints or using data from multi-shell acquisition are proposed to stabilize the fitting, but none of them restricts the diffusion tensor D to be positive definite. In this work, we formulate the bi-tensor model fitting as an optimization problem over the space of symmetric positive definite matrices and show that the objective function is a ratio of two geodesically convex functions. We also demonstrate by simulation that multi-shell data are needed for unbiased fitting of free water model in the presence of noise. Inspired by the Cholesky decomposition, D is treated as the product LL^T. The optimization is performed on L which guarantees the positive definiteness of D. Our model are evaluated with both simulations and real human brain data. Results show that the model is computationally efficient and the two-shell acquisition gives the best estimation.

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CP4

Quantum Density Operator Estimation

The quantum density operator is the fundamental element of quantum statistical mechanics. In this talk we use online estimation of the density operator via the metric projection onto the closed convex set of density operators in the Hilbert space of trace class operators. We will show existence of the projection and asymptotic convergence to the true density operator of a given quantum system.

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CP4

Kyle-Back Models with Risk Aversion and Non-Gaussian Beliefs

In this talk, we show that the existence of equilibrium in the Kyle-Back models can be characterized by considering a system of forward Fokker-Planck equation and a system of backward quasilinear parabolic partial differential equations coupled via an optimal transport type constraint at maturity. We also study the properties of the equilibrium in our model, where the insider is risk averse and the market maker's belief on the distribution of the price at final time is allowed to be non-gaussian.

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CP4

Eigendecompositions for Thermal Nondestructive Evaluation

Well known physical models govern the most common US Air Force nondestructive evaluation techniques (thermography, eddy current and ultrasound); however, the approximation of these models are neither fast nor accurate enough to use in many realistic nondestructive evaluation (NDE) scenarios. Inverse scattering and related approaches assumptions are not applicable in many NDE scenarios. Deviations from idealized systems caused by imperfections and other realism in experimental scenarios have a significant effect on the signals which can result in bias in the estimation of the damage extent. We present an approach that uses eigendecompositions to obtain a linear time invariant control system whose identification can be related to the geometry of the sample with inverse spectral geometry. In the example of thermography, we decompose the input signal (flash heat on the boundary) into Steklov eigenfunctions and the temperature throughout the domain into the relevant Robin eigenfunctions. The observed temperature on the boundary is also decomposed into a Steklov eigenfunction basis. We discuss the choices of underlying mixed Steklov-Neumann eigenfunctions, their effect on the structure of the matrices in the linear time invariant control system, and the identifiability of the system.

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CP4

A Discontinuous Galerkin Method for Wave Equations on Curved Geometries with Dirac Delta Source Terms

Linear wave equations with source terms containing Dirac delta functions and their derivatives occur in many areas of physics. For example, in extreme mass ratio binary (EMRB) systems solving the full Einstein equation is currently impossible, and a tractable approach is to linearize the equation around a non-flat geometry. The resulting wave equation is defined on a curved geometry and sourced by Dirac delta functions of potentially many derivatives. We develop a spectrally-convergent Discontinuous Galerkin method to numerically solve such wave equations. As proof of concept, we apply our method to an ordinary wave equation sourced by arbitrary nth-order derivatives of a Dirac delta function and a scalar wave equation defined on a Kerr geometry.

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CP4

Heat Dissipation Performance of Microchannel Heat Sink with Various Protrusion Designs

This research will focus on studying the effect of aperture size and shape of the microchannel heat sink on heat dissipation performance for chip cooling. The microchannel heat sink is considered to be a porous medium with fluid subject inter-facial convection. Derivation based on energy equation gives a set of governing partial differential equations describing the heat transfer through the microchannels. Numerical simulation, including steady-state thermal analysis based on CFD software, is used to create a finite element solver to tackle the derived partial differential equations with properly defined boundary conditions related to temperature. After simulating three types of heat sinks with various protrusion designs including microchannels fins, curly microchannels fins, and Micro-pin fins, the result shows that the heat sink with the maximum contact area per unit volume will have the best heat dissipation performance, we will interpret the result by using the volume averaging theorem on the porous medium model of the heat sink.

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CP5

Optimal Incentives to Mitigate Epidemics: A Stackelberg Mean Field Game Approach

Motivated by the models of epidemic control in large populations, we consider a Stackelberg mean field game model between a principal (regulator) and a mean field of agents evolving on a finite state space. The agents play a noncooperative game in which they can control their transition rates between states to minimize an individual cost. The principal can influence the resulting Nash equilibrium through incentives in order to optimize its own objective. We analyze this game using a probabilistic approach. We propose an application to an epidemic model of Susceptible-Infected-Recovered (SIR) type in which the agents control their interaction rate, and the principal is a regulator acting with non-pharmaceutical interventions such as making mask wearing mandatory or starting a quarantine. To compute the solutions, we propose an innovative numerical approach based on Monte Carlo simulations and machine learning tools for stochastic optimization. We conclude with numerical experiments by illustrating the impact of the agents' and the regulator's optimal decisions in two models: a basic SIR model with semi-explicit solutions and a more complex model which incorporates more states that we make use of the proposed numerical approach to find the Stackelberg Equilibrium.

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CP5

A Projection Method for Porous Media Simulation

Flow through porous, elastically deforming media is present in a variety of natural contexts ranging from large geophysical systems to biological contexts on cellular scales. When flow is approximated as incompressible, pore pressure acts as a Lagrange multiplier working to satisfy the resulting constraint on fluid divergence. Often, this yields a saddle-point problem requiring specialized preconditioners to solve efficiently. In this talk, we present a method for the simulation of flow through porous media and its coupled elastic deformation. The pore pressure field is calculated at each time step by projecting an intermediate mass-averaged material flux field onto a space of permissible functions in a manner similar to the Chorin projection method for incompressible flow. The corresponding linear system over the pressure space can be solved quickly at each time step using a geometric multigrid method due to the system's favorable properties. We will introduce the method and demonstrate its application to two- and three-dimensional systems arising in gel, mixture, and poroelastic theory.

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CP5

Thermodynamics of Turbulence

This talk concerns the physics of earthquakes and tsunamis, in the context of thermodynamics of turbulence. First, a background is discussed in terms of linear and convex analysis, and PDEs and stochastic PDEs. This is considered within the framework of Monte Carlo simulations, and how to improve these simulations when mean field theory is utilized (in context of scalar fields). After discussing the physics of this situation, Landau theory will be considered to extend mean field theory. Then, we will consider the context of renormalization group theory, and nonlinear scaling fields to go beyond mean field theory. Pade approximants and differential approximants will be discussed as bearing on calibrating Monte Carlo simulations, as simple examples of a renormalization group approach. We are using the geophysical framework of earthquakes/tsunamis for discussing thermodynamics of turbulence, as it is simple (i.e. scalar fields are useful) and the theory and experimental information is very extensive and well-known.

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CP5

A Natural Disasters Index

Natural disasters, such as tornadoes, floods, and wildfire pose risks to life and property, requiring the intervention of insurance corporations. One of the most visible consequences of changing climate is an increase in the intensity and frequency of extreme weather events. The relative strengths of these disasters are far beyond the habitual seasonal maxima, often resulting in subsequent increases in property losses. Thus, insurance policies should be modified to endure increasingly volatile catastrophic weather events. We propose a Natural Disasters Index (NDI) for the property losses caused by natural disasters in the United States based on the "Storm Data" published by the National Oceanic and Atmospheric Administration. The proposed NDI is an attempt to construct a financial instrument for hedging the intrinsic risk. The NDI is intended to forecast the degree of future risk that could forewarn the insurers and corporations allowing them to transfer insurance risk to capital market investors. This index could also be modified to other regions and countries.

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CP5

A Lattice Boltzmann Implementation of the Reference Map Technique for FluidStructure Interaction

We present a fully Eulerian simulation approach (LBRMT) for fluidstructure interaction (FSI) based on the reference map technique (RMT) and the lattice Boltzmann (LB) method. The new hybrid method provides an easy implementation of simulating the interaction between one or more deformable solids with a fluid on a single fixed mesh. It utilizes a blur zone from a level set function to construct a uniform continuous description of the solidfluid interface. We also introduce a new flux correction to the blur zone, which modifies the LB populations to preserve the solid and fluid density difference. The method also simplifies the inter-phase coupling with the collective advantages of the two Eulerian-based methods: the RMT computes the effect of solid stress, which is then passed on to the LB method as external force density to update fluid kinematics and solid deformation via a mesoscopic view of particle motion. Examples of incompressible neo-Hookean solids undergoing large deformation within a quasi-incompressible NavierStokes fluid show this method is flexible and robust in handling a range of FSI simulations. The LBRMT is suitable for simulating the bending, twisting, actuating, and sedimenting of arbitrary-shaped solids in a fluid.

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CP6

Numerical Approximations of Fractional Powers of the Laplace-Beltrami Operator

Several algorithms are available for the numerical approximations of fractional powers of elliptic operators. In this talk we focus on the method introduced which is based on a Balakrishan integral representation. An exponentially convergent sinc quadrature is applied to the latter leading to sequences of reaction diffusion problems approximated by standard finite element methods. This technology is applied to Laplace-Beltrami problems on closed surfaces as prototype for nonlocal elliptic problems on surfaces. The reaction-diffusion problems resulting from the sinc quadrature are approximated using parametric finite element methods. In this context, two sources of errors must be accounted for: the surface approximation error and the finite element approximation error on approximate surfaces. Our analysis requires optimal space discretization errors simultaneously in H^1 and in L^2. While the geometric error is inconsequential in H^1, it must be addressed with care in L^2. We discuss the intricate role of the geometric approximation and provide numerical simulations complementing the optimal rate of convergence obtained analytically.

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CP6

Experimental Estimation of a Sequence's Order of Convergence

A common technique in numerical analysis is to approximate a number L via some sort of iterative process, leading to a sequence of estimates x_n that (hopefully) approach L as n increases. A sequence's order of convergence p indicates how fast $x_n \to L$; in general, p indicates the approximate number of significant figures gained in x_n from one iteration to the next. If p=1 (linear convergence), the correct number of significant figures at each iteration is approximately an arithmetic sequence; for $p > 1$ (superlinear convergence), the correct number of significant figures at each iteration is approximately a geometric sequence. Let $e_n = |x_n - L|$ be the error in x_n. Formally, the order of convergence p is the number for which $\lim_{n\to\infty} \frac{e_{n+1}}{(e_n)^p} = \lambda$ for some constant λ. Given a sequence x_n of approximations, I discuss a novel method for approximating p and λ. These estimates can be useful when trying to accelerate convergence of a sequence, either directly as part of the accelerated method (e.g., bootstrapped Newton's method) or indirectly in trying to decide which acceleration method to use (e.g., Steffensen vs. Aitken acceleration). I give a derivation of the approximation formulas as well as several examples illustrating their performance.

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CP6

Least Squares Formulas - The Swiss Army Knife of Numerical Integration?

Least squares formulas were introduced by Wilson in 1970 to construct stable high-order quadrature formulas with equidistant points. The decisive idea behind these formulas is to allow the number of data points to be larger than the number of basis functions that can be treated exactly. This corresponds to the exact integration of a least squares approximation—rather than an interpolation polynomial—of the (unknown) integrand. In this talk, it is demonstrated how the concept of least squares formulas can also be used to tackle a myriad of other challenges in the context of numerical integration. These include the treatment of general weight functions (with mixed signs), numerical integration of experimental data, and the construction of positive interpolatory cubature formulas for general domains and weight functions.

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CP6

Conformal Accelerations Method and Efficient Numerical Solution of Boundary Problems for Fractional Differential Equations

We suggest a general framework for study of fractional differential equations in analysis and probability and a general methodology for efficient numerical solution of several types of boundary problems for fractional differential equations. Exact formulas using the Fourier/Laplace inversion and Wiener-Hopf factorization are derived. The resulting integrals are calculated numerically using appropriate conformal deformations of the contours of integration and the corresponding changes of variables, which greatly increases the rate of the decay of the integrals at infinity; then the simplified trapezoid rule is applied. The exponential rate of decay of the discretization error of the infinite trapezoid rule allows one to satisfy a small error tolerance with a moderate number of terms in the simplified trapezoid rule.

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CP6

Asymptotic Green's Function Methods for Time-Dependent Schrödinger Equations

Numerical simulation of the time-dependent Schrödinger equations is important in various applications. But it is challenging with conventional methods based on discretization of the equation on a mesh/grid, mainly due to that the domain is generally infinite and the wavefunction is highly oscillatory. Therefore, alternative methods are desirable. With the help of the perfectly matched layer method, the computation can be restricted to a bounded domain of special physical interest. Following that, the wavefunction will be propagated through Huygens' principle or Feynman's path integral, where an integral with the retarded Green's function is involved. The semi-classical approximation will be applied to approximate the retarded Green's function for a short period of time such that the integral can be evaluated to propagate the wavefunction for a short period of time. And the propagation can be repeated to a long time by use of the semi-group property. Appropriate low-rank approximations can be designed to approximate the integral such that it can be evaluated by the fast Fourier transform, which results in an efficient time propagator, based on asymptotic Green's functions, for the wavefunction. Numerical experiments will be presented to demonstrate the efficiency and accuracy of the asymptotic Green's functions method.

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CP6

Analytic Solutions for Inequality Constrained

Quadratic Programs.

Harry Markowitz transformed finance by framing portfolio construction as a trade-off between the mean and the variance of return, i.e., as a quadratic program. Variants of these optimization problems are frequently used for equity investment within the financial industry. For example, they form the basis for several prominent exchange traded funds that hold billions in net assets. It is well-known that when the portfolio weights face inequality constraints, as they do in practice, a numerical solver must be used. No general analytical results nor closed-form formulae appear in the literature. We develop analytic formulae for the solutions to quadratic programs that are constrained to lie on the standard simplex, and for which currently, only numerical solvers are applicable. Our approach makes use of fixed point theory to characterize the solution in a way that reveals its geometry. The obtained formulas lead to several results pertaining to the perturbation analysis of quadratic optimization problems. We discuss the implications of our work for portfolio problems in finance. When the quadratic form has a factor structure, our formulae also yield highly efficient algorithms. We analyze the complexity of these algorithms, develop a corresponding convergence theory, and benchmark their performance against state-of-the-art solvers on large portfolio problems.

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CP7

Asymptotic Solution of the Rayleigh Stability Equation: Application to the Growth of Wind Waves

When wind blows over water, ripples are generated on the water surface. In the framework of hydrodynamic stability, these ripples can be regarded as perturbations of the wind field, which is modeled by a parallel inviscid flow. For a given wavenumber k, the perturbed streamfunction of the wind field and the complex phase speed are the eigenfunction and the eigenvalue of the so-called Rayleigh equation in a semi-infinite domain. Because of the small air-water density ratio, $\epsilon \ll 1$, the wind and the ripples are weakly coupled. Hence, the eigenvalue problem can be solved perturbatively. At the leading order, the eigenvalue is equal to the phase speed c of surface waves. At order ϵ, the eigenvalue has a non-zero imaginary part, which implies growth. The growth rate is proportional to the square modulus of the leading order eigenfunction evaluated at the height $z = z_c$, where the wind speed is equal to c. In the limit of short and long waves, we construct uniform asymptotic approximations of the leading order eigenfunction. For short waves, an internal boundary layer of thickness $\sim 1/k$ emerges from the singularity, showing the dominant location of the wind-wave interaction. The long wave asymptotics provide a physical interpretation of the maximum growth rate. The results are confirmed using a numerical scheme, based on the integration of the Frobenius series about the regular singular point z_c, to compute this eigenfunction for a smooth wind profile.

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CP7

A Numerical Method for Self-Similar Solutions of the Ideal Magnetohydrodynamics

We present a numerical method to obtain self-similar solutions of the ideal magnetohydrodynamics (MHD) equations. Under a self-similar transformation, the initial value problem (IVP) is converted into a boundary value problem (BVP) by eliminating the time and transforming the system to self-similar coordinates [Samtaney, J. Comput. Phys. 1997]. The ideal MHD system of equations is augmented by a generalized Lagrange multiplier (GLM) yielding a mixed hyperbolic/parabolic correction to maintain the solenoidal condition on the magnetic field. The self-similar solution to the BVP is solved using an iterative method, and implemented using the P4est adaptive mesh framework. Existing Riemann solvers (e.g., Roe, HLLD, etc.) can be modified in a relatively straightforward manner and used in the present method. Extensive numerical tests illustrate that the present self-similar solution to the BVP exhibits sharper discontinuities than the corresponding one solved by the IVP. In problems with the presence of vortex sheets, the self-similar system results in a well-posed system compared with the IVP which exhibits a lack of convergence with mesh refinement. The present method is employed to investigate MHD shock refraction at a density interface [Wheatley et al. J. Fluid Mech, 2005]. In particular, we explore the parameter space of irregular shock refraction.

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CP7

Microswimmers near Deformable Interfaces

Unlike their passive counterparts, active microscopic swimmers at low *Re* exhibit interesting responses in confinement. For example, the response of "pusher" type microswimmers, such as bacteria *E.coli* or *B.subtilis*, varies from preferentially accumulating in the vicinity of plane boundaries (even in the dilute suspension limit) to a confinement-dependent emergence of complex spatiotemporal patterns in more dense suspensions. The dynamics of such systems depends crucially on the nature of the intervening boundary; namely free-slip versus no-slip, in case of plane boundaries, or non-deforming versus deforming interfaces. We present an analysis of the latter case involving the coupled hydrodynamics of a dilute suspension of microswimmers in the vicinity of a deformable interface. In particular, we characterize the nature of the membrane deformation and the resulting hydrodynamic stresses that emerge in the system. The analysis takes into consideration the role of the swimmer type (pusher or puller), the finite swimmer size and interface deformation due to surface tension as well as resistance to bending. We highlight the non-trivial ways in which the local and non-local effects influence the pressure force across the interface.

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CP7

Effects of Asymmetric Velocity Boundary Conditions in Rotating Rayleigh-Bnard Convection

A horizontally unbounded rotating layer of Boussinesq fluid begins to convect when an imposed adverse temperature gradient across its depth (characterised by the Rayleigh number, Ra) is sufficient to overcome the stabilising effects of rotation. However, if the boundaries in such a system obey a no-slip velocity condition, the net vertical heat transfer across the convecting layer can exceed that of a non-rotating layer with same Rayleigh number. This phenomenon is due to the Ekman pumping that occurs at the no-slip boundaries and has been observed in experiments and numerical simulations. The effect is enhanced for larger fluid Prandtl numbers and is absent if the boundaries are stress-free. When only one of the boundaries is stress-free, the vertical symmetry of the system is broken with Ekman pumping only occurring at the no-slip boundary. We study this situation numerically in an aspect ratio 2 system with a hot no-slip lower boundary and a cold stress-free upper boundary. We find that the enhanced heat transport discussed above vanishes and examine the role of the velocity and thermal boundary conditions in determining the mean temperature in the bulk and the mean heat transport.

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CP7

Steklov-Poincar Metric Based Shape Optimization for Fluid Mechanics

Shape optimization has enjoyed active research for decades due to its many applications, particularly in engineering. In order to solve a shape optimization problem, the concept of shape derivatives is needed. These can be expressed in so-called weak or strong forms, with the weak formulation being mostly preferred. The strong form, also known as the Hadamard form of the shape derivative, requires higher regularity of the state and adjoint variables related to the shape optimization problem. Additionally, the weak formulation arises automatically during the derivation of the strong form and requires less computational effort. We solve the shape optimization problem for a two-dimensional fluid-mechanical problem assuming a frictionless incompressible viscous fluid (Stokes flow) by presenting an optimization approach based on the Steklov-Poincaré metric, which allows us to use the weak shape derivative formulation. We present implementation details and numerical results of the aforementioned shape optimization problem of minimizing the viscous energy dissipation in Stokes flow, with multiple shapes being present in the computational domain and being optimised simultaneously.

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CP7

Deep Neural Network Enhanced Phase-Field Model for Fluid-Structure Interaction

Abstract: Phase-field approach can be used to model a multi-physics system, i.e., tumor growth, fluid-structure interaction, and multiple-phase flow. However, it is difficult to calibrate parameters or operator for the potential in a phase-field model. Deep neural network (NN) has shown power in inferring parameters and learning nonlinear continuous operator. We train a deep neural network to infer parameters and learn operators in phase-field model using synthetic data generated from both numerical simulations and experiments. We demonstrate that deep neural network is effective in inferring parameters and learning operators and complement a physical model.

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CP8

Far-Field Boundary Conditions for Simulating a 'patch' of Wall-Bounded Turbulent Flow

Wall-bounded turbulent flow is ubiquitous in nature. The near-wall region is a primary source of vorticity, energy dissipation, and turbulent kinetic energy, but it is asymptotically small compared to the bulk flow region. Hence it is difficult to access both experimentally and computationally. To better understand the near-wall dynamics, we formulate numerical simulations of the incompressible Navier-Stokes equations in a domain localized to the wall. The goal is to isolate the near-wall processes and model the effect of momentum transport from the bulk flow. Since the physical size of the domain decreases with the bulk flow Reynolds number, the computational cost is greatly reduced from direct numerical simulation (DNS). A significant challenge to overcome with this approach, however, is the need to pose boundary conditions at the non-physical computational boundaries. Our solution is to increase the size of the domain in the wall-normal direction to include a 'fringe' region, inside which the forcing is increased to provide momentum transport. Extensive comparisons to large-scale DNS validate the approach.

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CP8

The Moving Discontinuous Galerkin Method with Interface Condition Enforcement for Shock Dynamics with Material Strength Models

We extend the Moving Discontinuous Galerkin Method with Interface Condition Enforcement formulation to include material strength. In this work, we consider a discretized form of the Godunov-Peshkov-Romenski hyperelastic-type model. Additionally, a Jaumann rate hypoelastic-type model is investigated. We motivate this work by considering explicit shock-capturing schemes for these types of models which tend to produce smeared elastic and plastic shock waves. MDG-ICE resolves these discontinuities sharply, and maintains high order accuracy. MDG-ICE achieves this by fitting the elastic and plastic shock waves to space-time cell interfaces through interface condition enforcement, thereby allowing us to obtain non-oscillatory solutions without the use of limiters. We achieve accurate high order solutions even with relatively low mesh resolution. In this talk, we discuss the challenges of extending current formulations for fluid dynamics to include material strength, such as the derivation of jump conditions for the material strength models. We then demonstrate the ability of the MDG-ICE scheme to capture elastic and plastic shockwaves in a flyer impact problem. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, and funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 19-ERD-015.

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CP8

Nitsche-Type Unfitted Fluid Structure Interaction Model Coupled with Material Point Method

We propose a novel hybrid method that incorporates the Arbitrary Lagrangian-Eulerian (ALE) approach into material point method(MPM) for fluid-structure interaction(FSI) problems. In this formulation, fluid motion is described by Navier- Stokes equations formulated in ALE form. Variational formulation concerning the fluid is supported by the stabilizing residual-based variational multiscale(RBVM) method. Variational structural equations concerning the solid are assembled using MPM. We let fluid-solid interface cut the elements arbitrarily. To ensure well system conditioning and stability of the resulting system irrespective of how the interface intersects the cut elements, face-oriented ghost penalty stabilization is applied on the cut element faces. Continuity of velocities and normal stresses on the boundary is weakly enforced by the Nitsche's method. The advantage of our hybrid approach is that it provides a dynamic framework which eliminates certain shortcomings of ALE based finite element methods for fluid structure interaction problems involving large structural deformation. This study is supported by supported by NSF DMS Grant: Hybrid Fluid-Structure Interaction Material Point Method with applications to Large Deformation Problems in Hemodynamics.

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CP8

Analysis of a Space-Time Hybridized Discontinuous Galerkin Method for the Incompressible Navier-Stokes Equations

Much of the recent progress in the numerical solution of incompressible flow problems has concentrated on pressure-robust finite elements, a class of mimetic methods that preserve a fundamental invariance property of the incompressible Navier-Stokes equations. Two ingredients are essential for pressure-robustness: exact enforcement of the incompressibility constraint, and $H(\mathrm{div})$-conformity of the finite element solution. In this talk, I will introduce a space-time hybridized discontinuous Galerkin (dG) finite element method for the evolutionary incompressible Navier-Stokes equations. The method has a number of desirable properties, including point-wise mass conservation, energy stability, and higher-order accuracy in both space and time. Through the judicious use of a pressure facet variable, $H(\mathrm{div})$-conformity of the discrete velocity is enforced resulting in a pressure-robust method. Well-posedness of the resulting nonlinear algebraic system will be considered. Existence of the discrete solution is resolved in both two and three spatial dimensions using a topological degree argument, while uniqueness of the discrete solution is shown in two spatial dimensions under a small data assumption. Next, a priori error estimates for smooth solutions will be presented, as well as convergence to (Leray-Hopf) weak solutions using compactness theory for dG methods. Finally, the extension of the method to time-dependent domains will be discussed.

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CP8

On Imex-Afc Continuous Finite Element Methods for Visco-Resistive Mhd

In this work, a stabilized continuous finite element method for viscous and resistive magnetohydrodynamics is presented. This method is based on nodal variation limiting for algebraic flux correction schemes for hyperbolic systems. The resistivity and viscosity require the use of implicit time stepping. Thus, a nonlinear solver is used in which a Jacobian has to be constructed. With many time steppers, this demands that the limiting strategy be sufficiently differentiable, or that an approximate Jacobian be used. To relax this condition, IMEX time steppers are used in which the viscosity and resistivity are treated implicitly and the convection and stabilization are treated explicitly. Thus, fully accurate Jacobians are built resulting in a more robust solver. Some numerical examples are considered to demonstrate the performance of the method.

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CP8

Finite Element Approximation of Dirichlet Control using Boundary Penalty Method for Unsteady Magnetohydrodynamics

In this paper the author addresses a problem of optimal control of the magnetohydrodynamic equations with Dirichlet boundary conditions on the flow velocity, utilizing a penalty approach, which leads to more easily implementable boundary conditions for the adjoint equations than the conventional ones. The rigorous mathematical analysis presented in this paper provides well-posedness of the penalized problem. In addition, a finite element method of the mixed Galerkin type is applied to its numerical approximation, which leads to error estimates for both the primal and adjoint variables. Furthermore, the numerical method is applied to a non-trivial computational test of controlling a flow with a recirculation, which demonstrates its usefulness.

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CP9

Convergence Analysis for a High-Order Compact Schemes for the Buckling and the Clamped Plate Problems: a New Approach

We propose a new approach for the analysis of high-order compact schemes for the buckling and for the clamped plate problems. In our book, we have suggested a fourth-order compact scheme for the Navier-Stokes equations. The buckling plate problem in 2D, $\partial_t \Delta u = \Delta^2 u + f$, contains all the linear components of the NS equations in streamfunction formulation. For these methods the truncation error is only of first-order at near-boundary points, but is of fourth order at interior points. Invoking a suitable matrix analysis, we prove that the convergence rate is actually four. Thus, the error tends to zero as $O(h^4)$, where h is the size of the mesh. We analyzed a two-dimensional model for the clamped plate problem. Here we extend the analysis to a problem containing lower order derivatives and prove that in this case too the error is $O(h^4)$. Numerical results demonstrate fourth-order convergence rates.

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CP9

Low Mach Number Asymptotic Analysis of Artificial Diffusion in Model Numerical Schemes

Simulating low Mach number flows, both with and without acoustics, is important in many areas of physics and engineering. Collocated, density-based numerical schemes are widely used in computational fluid dynamics due to their geometric flexibility and their applicability across moderate Mach numbers. However, standard schemes of this type are known to fail at low Mach number, so special care must be taken when designing schemes that are uniformly accurate across a wide Mach number range. Previous analyses usually consider only whether the discrete form of one particular scheme, or a very restricted class of schemes, is suitable for low Mach number simulations without acoustic effects. We augment the continuous Euler equations with artificial diffusion terms, producing modified equations which are representative of a wide class of discretisation schemes. Using single- and multiple-scale asymptotic analyses, we find constraints on the artificial diffusion for flows either with or without acoustic effects. We are able to reproduce, at the continuous level, several known properties of discrete low Mach number schemes, as well as shed light on the causes of several numerical instabilities previously reported in the literature. This approach allows analysis and design of a broad class of low Mach number numerical schemes independently of the specific discretisation, and could lead to novel strategies for preventing the discussed numerical instabilities.

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CP9

Nonoverlapping Domain Decomposition Smoothers for $3D$ $H(\mathbf{curl})$ Problems

We suggest a multigrid method for problems arising from edge elements. Since the conventional smoothers do not work well, a new type of smoothing method is essential for solving vector field problems. We introduce new smoothing techniques based on nonoverlapping domain decomposition preconditioners. The smoothers play a main in multigrid methods for solving problems posed in $H(\mathbf{curl})$.

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CP9

A Multi-Scale Iterative Approach for Completion

of Missing Data Entries

A common pre-processing task in machine learning is handling missing data entries, also known as imputation. Standard techniques use mean values, regression or optimization based techniques for predicting the missing data values. In this work, a kernel based technique is utilized for imputing data in a multi-scale manner. The construction is based on Laplacian pyramids, which operate on the row and column spaces of the data in several scales. Experimental results demonstrate the approach on publicly available datasets, and highlight its simple computational construction and convergence stability.

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CP9

A Moving Mesh Finite Element Method for Modelling Defects in Liquid Crystals

Defects in a liquid crystal director field can arise due to external factors such as applied electric or magnetic fields, or the constraining geometry of the cell containing the liquid crystal material. Understanding the formation and dynamics of defects is important in the design and control of liquid crystal devices, and poses significant challenges for numerical modelling. In this talk we consider the numerical solution of a Q-tensor model of a nematic liquid crystal, where defects arise through rapid changes in the Q-tensor over a very small physical region in relation to the dimensions of the liquid crystal device. The efficient solution of the resulting six coupled partial differential equations is achieved using a finite element based adaptive moving mesh approach, where an unstructured triangular mesh is adapted towards high activity regions, including those around defects. Spatial convergence studies show the adaptive method to be optimally convergent using quadratic triangular finite elements. The full effectiveness of the method can be seen when solving a challenging two-dimensional dynamic Pi-cell problem involving the creation, movement, and annihilation of defects.

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CP9

Goal-Adaptive Meshing for Non-Linear Isogeometric Shell Analysis

The idea behind Isogeometric Analysis (IgA) is to enable seamless integration between Computer-Aided Design (CAD) and numerical analysis by employing the spline basis functions for geometric representation in CAD in the analysis. Applications of IgA include structural analysis problems amongst other disciplines. In some structural analysis applications, for example fatigue analysis, accurate descriptions of stress fields are of importance to predict structural safety. Accurate description of these fields are enabled by the higher-order continuity of the basis functions in isogeometric shells. To balance computational costs and accuracy, adaptive meshing can be employed. Elements are typically refined based on their contribution to the total error measure [A. Buffa et al.,Adaptive isogeometric methods with hierarchical splines: Error estimator and convergence,2016]. We employ the Dual-Weighted Residual method [R. Rannacher,Adaptive finite element methods in flow computations,2004] to compute element-wise error contributions with respect to a goal functional (e.g. a stress measure) and Truncaded Hierarchical B-splines [C. Giannelli et al., THB-splines: The truncated basis for hierarchical splines,2012] to provide local mesh refinements. We evaluate different goal functionals for both (non-)linear equilibrium analyses (i.e. static or dynamic analysis) as well as eigenvalue analyses (i.e. buckling analysis) and assess their effectivity for different problems.

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CP10

A New Sir Model with Mobility

In this paper, an SIR (Susceptible- Infectious- Recovered) model with mobility will be studied. A traditional SIR model used in epidemiology describes the transition of particles among states, such as susceptible, infected, and recovered states. However, the traditional model has no movement of particles. There are many variations of SIR models when it comes to the factor of mobility, the majority of studies use mobility intensity or population density as a measure of mobility. In this paper, a new dynamical SIR model, including the spatial motion of three-type particles, is constructed and the long-time behavior of the first and second moments of this dynamical system are studied.

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CP10

Network Evolution Models under Triadic Closure: Hierarchy and Bistability.

In this work, we aim to present a hierarchy of network evolution models under the triadic closure, based on the work by Grindrod, Higham and Parsons [Internet Mathematics, 8, 2012, 402-423]. In the existing literature, it has experimentally been derived how triadic closure effects can lead to bistability in the formation of social interaction networks and, hence, based on the initial conditions and transient dynamics, the system may evolve towards either of two long-time states. In our work, we rigorously show that, in a macroscale regime, the bistability phenomenon is admitted, i.e., the steady state is bimodal, and hence a typical solution trajectory alternately spends time close to two distinct levels and we analyze how some features of the system are shared by the different models. Selected numerical experiments are provided to confirm the theoretical analysis. This is joint work with Desmond John Higham and Kostantinos Zygalakis (University of Edinburgh).

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CP10

Forward-Backward-Half Forward Dynamical Systems for Monotone Inclusion Problems

In this work, we investigate first order forward-backward-half forward dynamical systems associated with an inclusion problem consisting of the sum of three monotone operators in a real Hilbert space framework. We study the existence, uniqueness, and weak asymptotic convergence of the generated trajectories. We have provided a variable metric forward-backward-half forward dynamical system in the sense of non-self-adjoint linear operators and also analyzed the case in which linear operators depend on time. Also, this idea permits us to extend the forward-backward-forward dynamical system and forward-backward dynamical system in the framework of variable metric and relaxes some conditions on the metrics.

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CP10

Complex Dynamics in Networks, Templates and Mutated Systems

We explore three directions extending the traditional theory of complex quadratic iterations: (1) complex quadratic networks; (2) template iterations and (3) mutated iterations. Broadly speaking, these address generalizations of single map quadratic iterations to the case where multiple variables are coupled as nodes in a self-interacting network, and to the case where the iterated map is subject to temporal and spacial errors in replication. Each direction is built towards addressing in a unified, canonical framework an essential open problem in neuroscience, genetics and medicine, respectively. In all three cases, the system's long-term dynamics is highly non-trivial, and can be represented by asymptotic sets (Mandelbrot and Julia sets) with specific topological signatures, and with properties far beyond those described in the case of single map iterations. Understanding the complexity of these sets requires a comprehensive mathematical approach, in which analytical and computational aspects are tightly combined.

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CP10

Complex Oscillatory Patterns As Long-Term Transient Dynamics in a Two-Timescale Ecosystem.

A two-trophic ecosystem comprising of two species of predators competing for their common prey with explicit interference competition is considered. With a proper rescaling, the model is portrayed as a singularly perturbed system with fast prey dynamics and slow dynamics of the predators. In a parameter regime near singular Hopf bifurcation, chaotic mixed-mode oscillations (MMOs) featuring concatenation of small and large-amplitude oscillations, which could persist for thousands of generations, are observed as long-term transient dynamics, before the system experiences a regime shift. To analyze the dynamical cause that initiates a large amplitude oscillation in an MMO orbit, the model is reduced to a suitable normal form near the singular-Hopf point. The analysis is used to determine whether a trajectory would exhibit another cycle of MMO dynamics before approaching its asymptotic state.

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CP10

A New Theory of Weak Fractional Calculus, Sobolev Spaces, and the Fractional Calculus of Variations

At the heart of this presentation is the introduction of the notion of weak fractional derivatives. An overview of their associated calculus (characterization theorem, product and chain rules, and the Fundament Theorem of Weak Fractional Calculus) will be given before exploring the development of new fractional Sobolev spaces. Unlike existing definitions, these spaces are analogous to the well understood integer order Sobolev spaces as they are defined through the notion of weak fractional derivatives. We will review key properties such as trace concept(s) and Sobolev embedding theorems, including a fractional Poincaré inequality. Using the developed machinery, we study well-posedness results of some model problems from the fractional calculus of variations. Moreover, special attention will be given to the consequences the developed theory has on fractional PDEs, including new fractional Laplacian(s), fractional Neumann boundary operator(s), and understanding how to pose Dirichlet boundary value problems.

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CP11

How Multi-Scale Modeling and Signal Processing Can Assist the Diagnosis of Pots

Postural Orthostatic Tachycardia Syndrome (POTS) is characterized by an increase in heart rate (tachycardia) upon the transition to an upright position. This syndrome is most common in young females, but has recently also been observed in patients with long-term effects of COVID. It has been hypothesized that POTS have increased baroreflex sensitivity possibly due to expression of agonistic antibodies binding to receptors on smooth muscle cells and the sinoatrial node. We use a multi-scale approach to explain POTS by: 1) Employing non-stationary signal processing to show that heart rate and arterial blood pressure oscillations in the low-frequency range, approximately 0.1 Hz, is enhanced in POTS patients when compared to controls. 2) The enhancement of these oscillations for POTS patients can be explained using a cardiovascular model with the baroreflex control modeled using first order kinetics. Increased baroreflex sensitivity is modeled by steepening the control curve for heart rate and peripheral vascular resistance. Moreover, by changing core parameters controlling blood volume and baroreflex response we are able to differentiate POTS sub-groups. 3) Finally, by coupling the cardiovascular model with a sinoatrial node cell model we are able to test if the presence of antibodies binding to specific receptors cause larger low-frequency heart rate and blood pressure oscillations.

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CP11

Oscillatory Dynamics in the Dilemma of Social Distancing

Social distancing as one of the main non-pharmaceutical interventions can help slow down the spread of diseases, like in the COVID-19 pandemic. Effective social distancing, unless enforced as drastic lockdowns and mandatory cordon sanitaire, requires consistent strict collective adherence. However, it remains unknown what the determinants for the resultant compliance of social distancing and their impact on disease mitigation are. Here, we incorporate into the epidemiological process with an evolutionary game theory model that governs the evolution of social distancing behaviour. In our model, we assume an individual acts in their best interest and their decisions are driven by adaptive social learning of the real-time risk of infection in comparison with the cost of social distancing. We find interesting oscillatory dynamics of social distancing accompanied with waves of infection. Moreover, the oscillatory dynamics are dampened with a non-trivial dependence on model parameters governing decision-makings and gradually cease when the cumulative infections exceed the herd immunity. Compared to the scenario without social distancing, we quantify the degree to which social distancing mitigates the epidemic and its dependence on individuals responsiveness and rationality in their behaviour changes. Our work offers new insights into leveraging human behavior in support of pandemic response.

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CP11

Usefulness of Machine-Learning-Predicted Probability As a New Risk Index for Prediction of Renal and Life Prognoses of Chronic Kidney Disease

[Background] Personalized prediction is useful for chronic kidney disease (CKD) therapy. Predialysis death is a competitive risk of dialysis in CKD patients and lowers the accuracies of the prediction of their prognoses. Thus, we determined whether machine-learning-predicted probability works as an index for both the risks and attempted its application. [Methods] We constructed a database of electronic-medical-record of CKD patients in Japan (15 university hospitals), and developed models using random forest (RF), Gradient Boosting and eXtreme Gradient Boosting for the prediction of dialysis and death over 1 year. Their performances were compared by bootstrap method with those of clinical indices, such as kidney-failure-risk equation (KFRE), which is one of the validated risk-prediction indices. [Results] 16 models showed high performances. Specifically, RF models including 22 or 8 variables showed high C-statistics: 0.916 (95% CI 0.88, 0.952) and 0.907 (0.863, 0.951), respectively, which were higher than KFRE (p¡0.0001). Cox proportional hazards models with spline showed the relationship between the probabilities and the outcome risks. We also developed a Web-based risk prediction system using those models, which was superior in practicality in a prospective CKD cohort study(n=67,957). [Conclusions] This study showed that the machine-learning-based probability is useful as a new risk index for dialysis and death and applicable to clinical practice.

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CP11

Computational Study of Sars-CoV-2 Infection Inhibitor Hydroxychloroquine on Cardiac Toxicity

The outbreak of coronavirus disease 2019 (COVID-19) poses a serious threat to global health and economies. With the heightened interest in the potential use of hydroxychloroquine (HCQ) to treat patients with SARS-CoV2, it may be prudent to reflect on the risks of therapy, particularly their cardiac toxicity. This computational study investigates the propensity of HCQ in causing bradycardia. The sinoatrial node (SAN) cell is presented as an equivalent electrical circuit comprising nine ion channels. All ionic currents are described by ordinary differential equations. An HCQ drug model for the hyperpolarizing-activated current or funny current i(f) is simulated after mining data from experimental studies. The resting membrane poten-

tial is set at -80mV. The steady-state value of the activation parameter of the funny current i(f) is shifted to the negative side after applying HQN of 1 M. The action potential (AP) timing is altered when we incorporated the biophysically modified i(f). The results show that the modified i(f) plays an important role in reducing the frequency of the spontaneous AP at the SA node. We simulated the effects of HCQ drug upon funny current and action potential. As hydroxychloroquine reduces the frequency rate of the spontaneous action potential firing, we should prevent it as a potential drug against COVID-19.

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CP11

An Agent-Based Model of Pain-Related Neural Activity in the Amygdala

In this talk, we present a computational modeling approach to understand and predict pain output from the amygdala, a part of the brain involved in stress adaptation, emotional regulation, and pain. We developed an agent-based model of two distinct inhibitory neuron populations in the amygdala, those that express protein kinase C delta (PKC) and those that express somatostatin (SOM). Within the model, a network of neural links simulates connectivity and the transmission of inhibitory signals between neurons. Type-specific parameters describing the response of these neurons to painful stimuli were estimated from published data as well as our own wet-lab experiments. The model outputs an abstract measure of pain, which is calculated in terms of the cumulative pro-nociceptive and anti-nociceptive activity across neurons in both hemispheres of the amygdala. Results demonstrate the ability of the model to produce changes in pain that are consistent with published studies and highlight the importance of several model parameters.

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CP11

Quantitative Reasoning and Computational Laboratories for Non-Majors Biology

We have developed a textbook, *Biology for the Global Citizen*, for a non-majors biology course that includes laboratory exercises using computer simulations. These exercises employ the scientific method, enhance quantitative literacy through interpretation of graphs and basic statistics with spreadsheets, employ data to support conclusions, emphasize critical thinking and analysis, and include questions that can be graded automatically and discussion questions. The simulations are written in the widely used agent-based simulation software, NetLogo, which is free, easy to use, and requires no programming experience. Guided by introductory videos and lab exercises, students consider various scenarios, make hypotheses, adjust variables to test the effect of each scenario, run simulations multiple times, generate and interpret data and graphs, make observations, draw conclusions, apply their conclusions to decision making, and gain a deeper understanding of the science that the model simulates. Besides exposing students to the third paradigm of science, computation, use of simulations enables students to perform experiments that are too difficult, time-consuming, costly, or dangerous to perform otherwise. The authors adapted and added models, such as the spread of COVID-19, to numerous models downloaded with NetLogo. After class testing at six institutions this year, the first edition will be available through Cognella Academic Publishing in the fall.

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CP12

GPU-Accelerated Quadrature Moment Methods

The population balance equation is a PDE used to model the evolution of disperse populations of particles. Quadrature moment methods (QMOMs) represent its solution in terms of a set of statistical moments by formulating corresponding moment-transport equations and closing them via quadrature. In physics-based simulations, the algorithms for converting the moment set to quadrature points and weights are computationally costly relative to the other operations performed (e.g. field derivative approximation). This cost increases for non-Gaussian statistics as more quadrature points and moments are required to maintain model accuracy. We propose a set of QMOM algorithms for GPUs that utilize the single-instruction/multiple-data (SIMD) character of the inversion routines, kernel task-parallelism and memory-transfer–compute overlap. These routines are shown to be computationally cheap when compared to their CPU counterparts, achieving speed-up by more than an order of magnitude for practical batch sizes. For many problems this speed-up makes the inversion algorithm comparable to or cheaper than typical derivative approximation algorithms.

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CP12

On Mathematical Modeling of Erosion and Deposition in Complex Porous Media

We study flow suspension featuring erosion and deposition of solid particles at a micro-scale level and their direct consequence on the geometrical structure formation. These processes are ubiquitous and can be found, for instance, naturally in the geological sedimentation and artificially in dams where the "piping" phenomenon often occurs. In this work, we formulate novel and idealized mathematical models to examine the internal evolution of flow-networks in a connected pore structure undergoing a unidirectional flow using asymptotic and numerical techniques. Starting from the Stokes equations combined with the advection-diffusion equation, we propose a model to construct a complete analysis of both the erosion and deposition in geological structures and porous media. The deposition-erosion model is of threshold laws: erosion and deposition occur when the total shear stress is, respectively, greater and lower than some specific critical values, depending on the solid material. Throughout this study, we investigate the networks' evolution, which hinges on 1) parametric research on specific types of membrane properties and their influence on the reconfiguration regime within the channel; and 2) a geometrical study addressing the intra-layer connectivity and its impact on the performance; subject to an imposed local concentration of particles. Using these approaches, we study channelization in the pore structure under constant flux and pressure-driven flow.

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CP12

On Optimizing the Performance of Pleated Membrane Filters

Pleated membrane filters are used in a variety of industrial applications, since they offer more surface area to volume ratio that is not found in equivalent flat filters. A pleated membrane filter consists of a porous membrane layer which is surrounded by two supporting layers. The whole structure is pleated and placed into a cylindrical cartridge. In this work, we introduce a novel 3D model of a pleated membrane filter that consists of a hollow, membrane, and empty regions. We also introduce the advection diffusion equation to our model which allows for further studies pertaining to the concentration of particles present in the pleated membrane filter. A mathematical model is developed using Stokes equation for the flow in the empty, hollow and support layer regions along side with Darcys law for the membrane. Using key assumptions based on small aspect ratios of the filter cartridge, the support layers, and the membrane pores, we can further simplify the flow within the pleated membrane filter as well as the particle concentration, such that the resulting equations can be solved with numerical methods. By performing these steps, we seek to discover an optimal pleat packing density to find the optimum filter performance, while not exceeding a threshold for the particle concentration at the filter outlet.

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CP12

Optimizing Pleated Filter Performance Based on Variable Pleat Packing Density

Pleated membrane filters consist of a membrane layer sandwiched between two support layers on either side that are all pleated together and surrounded around a cylindrical cartridge. This type of filter is widely used in many different applications due to offering a high ratio of filtration surface area to its volume. However, typically a pleated filter is not as efficient as a flat filter with equivalent surface area due to several possibilities such as damage of the membrane during the pleating process, the complex flow within the pleated membrane, or additional resistance from the pleat packing density. In this work, we focus on how the pleat packing density affects the filtration performance of a pleated filter, while extending the work from Sanaei et al. J. Fluid Mech. 2016 to investigate the performance of a 3D filter cartridge with a more detailed geometry accounting for axial variations and curvature of the cartridge. We model the flow in the cartridge using the Stokes equations and Darcy's law. The cartridge consists of an empty area for inflow, a pleated membrane, and a hollow region for outflow. By utilizing the small aspect ratio of the pleat length to the length of the cartridge, we are able to simplify the model using asymptotic analysis. From this, we can investigate how the performance of pleated membrane filters is affected by the pleat packing density in order to optimize the amount of pleats to achieve the optimum filtration performance.

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CP12

Integrating Trim Analysis into a Coupled Physics Workflow for Numerically Simulating Hypersonic Flight

One of the highest priorities within the current Department of Defense strategies is the design and analysis of hypersonic air vehicles. Numerical simulations that seek to represent the pertinent physics that describe hypersonic flight must include the coupled interactions of fluid dynamic forces, mechanical stresses, and thermal loadings on the vehicle of interest. For a maneuvering vehicle, the effects of the coupled physics interactions on the overall stability of the vehicle must be understood. Most notably, the trim state of the vehicle must be understood over a wide range of flight conditions. The trim state of a vehicle corresponds to the point where no force needs to be exerted manually to maintain stability. We are currently exploring various ways to integrate trim calculations into a coupled physics workflow that leverages high-fidelity numerical simulations of hypersonic flight. A trim analysis will be conducted to determine how mechanical and thermal deformations of the vehicle affect the overall trim state at various flight conditions. We will investigate how the convergence of the multi-physics solutions vary when trim is calculated both with and without the deformations imposed on the vehicle.

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CP12

The Effects of the Endothelial Surface Layer on Red Blood Cell Dynamics in Microvessel Bifurcations

Red blood cells (RBCs) make up 40-45% of blood and have an important role in oxygen transport. That role depends on their nonuniform distribution throughout the body which depends, in turn, on how RBCs are distributed at diverging vessel bifurcations (one vessel flows into two) and the presence of an endothelial glycocalyx or endothelial surface layer (ESL) that is 0.4-1 μm thick and lines vessel walls. The effects of the ESL on RBC deformation, distribution, and penetration into the ESL in a diverging capillary bifurcation is analyzed using a flexible, two-dimensional model. The RBC is represented using interconnected viscoelastic elements. Stokes flow equations (viscous flow) model the surrounding fluid. The ESL is modeled using the Brinkman approximation for porous media. One cell passes through the bifurcation at a time so there are no cell-cell interactions. A range of physiologically relevant hydraulic resistivities and osmotic pressures are explored. Decreasing hydraulic resistivity and/or decreasing osmotic pressure produced four behaviors: 1) RBC distribution nonuniformity increased; 2) RBC deformation decreased; 3) RBCs slowed down slightly; and 4) RBCs penetrated more deeply into the ESL. We will discuss how the altered flow profile and ESL resistance to penetration generated these behaviors. In certain scenarios, penetration was deep enough to raise the possibility of cell adhesion, as can occur in experiment in pathological situations.

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CP13

Upscaling Phase Transition Models with Applications to Permafrost Models

Permafrost is a dynamic environment ubiquitous in the Arctic, and we are interested in modeling its response to the climate controls, starting from the pore-scale of [mm] scale up to field scale of [m]. We start with a model for heat conduction and ice/water phase transitions in a domain composed of rock grains and water in liquid or solid phase, and consider next its numerical upscaling. Specifically, we consider phase field relaxation of the Stefan problem, a non-linear free boundary value problem. We discuss challenges of numerical approximation but focus on the upscaling of coefficients of the model as well as of the temperature-enthalpy relationship. We compare the upscaled results with field data used in Darcy scale models.

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CP13

Fast Summation Methods Based on Barycentric Lagrange Interpolation

We present two fast summation methods based on barycentric Lagrange interpolation for particle interactions. The first is a treecode (BLTC) and the second is a fast multipole method in which the interaction lists are formed by dual tree traversal (BLDTT). The BLTC uses particle-cluster approximations, while the BLDTT uses particle-cluster, cluster-particle, and cluster-cluster approximations. The methods are kernel-independent and a distributed memory implementation running on multiple GPUs has been developed. The performance of the BLTC and BLDTT is demonstrated for several particle systems.

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CP13

Scalable High-Order Time-Stepping via Krylov Subspace Spectral Methods

For time-dependent PDEs, both linear and nonlinear, Krylov Subspace Spectral (KSS) methods offer a balance between the efficiency of explicit methods and the stability of implicit methods, by computing each Fourier coefficient using techniques of Golub and Meurant for approximating bilinear forms. This talk will present recent developments with KSS methods, including applications to problems from acoustics, recent theoretical results pertaining to stability, and combination with fictitious domain methods for solving PDEs on general domains.

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CP13

A Multistep Spectral Method for Time-Dependent Pdes

Krylov subspace spectral (KSS) methods are high-order accurate, explicit time-stepping methods for partial differential equations (PDEs) with stability characteristic of implicit methods. Unlike other time-stepping approaches, KSS methods compute each Fourier coefficient of the solution from an individualized approximation of the solution operator of the PDE. As a result, KSS methods scale effectively to higher spatial resolution. This talk will present an explicit multistep formulation of KSS methods to provide a "best-of-both-worlds" situation that combines the efficiency of multistep methods with the stability and scalability of KSS methods. The effectiveness of the multistep KSS method will be demonstrated using numerical experiments.

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CP13

Numerical Solutions to the Free Boundary Problem for a Void in a Stressed Solid with Anisotropic Surface Energy

We consider the interaction of elastic stress and anisotropic surface energy on the shape of a void in an elastically-stressed solid. The void shape is a free-boundary problem determined by the minimization of elastic strain energy and surface energy. The equilibrium shape of the void has corners for sufficiently strong surface energy anisotropy, and the presence of corners will generate integrable singularities in the elastic stress. The contribution of these singularities to the total elastic strain energy can alter the entire void shape. We develop a numerical method for solving the free-boundary problem using a complex-variables boundary integral equation for the elasticity problem, coupled to a spectral method for determining the energy-minimizing shape. A novel feature of our work is the incorporation of an explicit corner term in the representation of the stress field that is derived from the asymptotic analysis of the corner region. Our results determine how the singularities associated with corners have a global effect on the entire shape of the void and affect the equilibrium corner angles on the void shape.

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CP13

Anderson Acceleration using the H^{-S} Norm and the Implicit Preconditioning Effects

Anderson acceleration (AA) is a technique for accelerating the convergence of fixed-point iterations. We propose the idea of applying AA to a sequence of functions and modify the norm in its internal optimization problem to the H^{-s} norm, for some integer s, to bias it towards low-frequency spectral content in the residual. The choice of s is to counterbalance the implicit spectral biasing in certain fixed-point operators. We rigorously analyze the convergence behavior of one-step AA, providing an explicit error bound using Chebyshev polynomials that decreases exponentially in the memory parameter m. Numerical experiments for both contractive, noncontractive, and non-linear operators demonstrate the acceleration effects of AA based on different norms. The idea belongs to the sequence of work examining the preconditioning and "implicit" regularization effects of different mathematical metrics as the objective function in optimization, as the likelihood function in Bayesian inference, and as the measure of residual in numerical solution to PDEs.

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CP14

Modeling the Risk of SARS-CoV-2 Transmission from Environmental Surfaces

Beginning in late 2019, the coronavirus disease (COVID-19), originating in Wuhan, China, quickly spread across the globe leading to one of the most devastating pandemics of the 21st century. While direct person-to-person transmission of SARS-CoV-2, the etiological agent of COVID-19, appears to be the primary route of transmission, the contraction of SARS-CoV-2 from various surfaces in the environment is also considered a potential contributor to the disease transmission as the infected individuals shed virus onto environmental surfaces through sneezing, coughing, and breathing. In this study, we develop a mathematical model to predict the probability of detecting SARS-CoV-2 in environmental reservoirs during the COVID-19 outbreak in a community. Furthermore, we extend our model to quantify the contribution of environmental virus to COVID-19 cases in a community. We validate our model using experimental data with a large number of swab samples collected from commonly touched surfaces across San Diego County. Our model, which is capable of describing transmission dynamics of COVID-19 within San Diego County, allows us to compute the risk for an individual to encounter virus in the environment. The results indicate that the persistence of virus on some environmental surfaces can significantly increase COVID-19 cases in a community.

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CP14

Biphasic Range Expansions with Short and Long-Distance Dispersal

Long-distance dispersal (LDD) has long been recognized as a key factor in determining rates of spread in biological invasions. Two approaches for incorporating LDD in mathematical models of spread are mixed dispersal and heavy-tailed dispersal. In this talk, I analyze integrodifference equation (IDE) models with mixed-dispersal kernels and fat-tailed (a subset of the heavy-tailed class) dispersal kernels to study how short- and long-distance dispersal contribute to the spread of invasive species. I show that both approaches can lead to biphasic range expansions, where an invasion has two distinct phases of spread. In the initial phase of spread, the invasion is controlled by short-distance dispersal. Long-distance dispersal boosts the speed of spread during the ultimate phase, and can have significant effects even when the probability of LDD is vanishingly small. For fat-tailed kernels, I introduce a method of characterizing the "shoulder' of a dispersal kernel based on speed rarefaction curves, which separates the peak and tail.

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CP14

Host-Parasitoid Dynamics and Climate-Driven Range Shifts

Climate change has created new and evolving environmental conditions that cause the habitat ranges of many species to shift upward in elevation and/or towards the poles. To investigate the impact of climate-driven range shifts on host and parasitoid insect species, I consider an integrodifference equation (IDE) model. Using this IDE model, I determine criteria for coexistence of the host and parasitoid species as the habitat shifts spatially. I compare several methods of determining the critical habitat speed, beyond which the parasitoid cannot survive. To make the analysis tractable, I determine the critical speed from a spatially-implicit model that uses an approximation of the dominant eigenvalue of an integral operator. Because the kernel is asymmetric, classical methods for determining the dominant eigenvalue perform poorly. Instead, I approximate the dominant eigenvalue with a method known as geometric symmetrization. The critical speed for parasitoid survival, as computed from the spatially-implicit model, is a good lower bound for the critical speed as determined from simulations of the full IDE model. This framework allows for further exploration of how biological factors impact the coexistence of the host and parasitoid species.

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CP14

Modeling the Invasion Wave of Wolbachia in Mosquitoes for Controlling Mosquitoes-Borne Diseases

We develop and analyze a partial differential equation (PDE) model to study the transmission and invasion dynamics of releasing Wolbachia-infected mosquitoes to establish infection among the wild uninfected mosquitoes. Wolbachia is a novel mitigation strategy to control mosquitoes-borne diseases, such as Zika, Chikungunya, and dengue fever. It is a natural bacterium that can infect mosquitoes and reduce their ability to transmit these diseases. A critical threshold condition that determines if a Wolbachia infection can be sustained in the wild is the ratio of infected to uninfected mosquitoes. Thus, accounting for the spatial heterogeneity in the distributions of the infected and uninfected mosquitoes is critical to accurately predict if a release can be sustained in the field. We create a reaction-diffusion type PDE model for the spread of a Wolbachia epidemic within the mosquito population. The model accounts for both the complex vertical transmission parameters (from different mosquito life-stages) and the horizontal transmission (spatial diffusion) of Wolbachia infection. We identify the spatial threshold condition for the Wolbachia invasion, beyond which the model can give rise to the traveling waves. The threshold is captured using a reduced 1-PDE model and further simulated using the 2-PDE model. We then compare the spatial threshold distribution to the previous ODE setting as well as other spatial configurations of the releasing profiles.

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CP14

Network Models for Analyzing the Deformities Induced by the Ecotoxicological Contaminant Tris(4-Chlorophenyl)Methanol (tcpmoh) in Developing Zebrafish (Danio Rerio)

Tris(4-cholophenyl)methanol (TCPMOH) is a recently discovered environmental water contaminant with an unknown origin. Although novel, it is highly persistent in the environment, bioaccumulates in marine species, and has been found in human breast milk. This study investigates the effects of TCPMOH using the zebrafish model (Danio rerio) by assessing TCPMOH induced deformities during the developmental stage. Zebrafish have been exposed to 0.0, 0.5, 1.0 or 5.0 M TCPMOH and monitored during the developmental stage by way of microscopy imaging. Morphological data has been gathered assessing deformities and mortality of each sample at 24-hour intervals. A complex network model has been developed to analyze the association between deformities and mortality within and between experimental groups using mathematical correlations and spectral decomposition analysis. The spectral radius for each network has been assessed and reveals morphological deformity associations and a statistically significant increase in deformities in exposed samples.. Node importance analysis reveals yolk edema is highly associated with the onset of other deformities and mortality. The findings of this study reveal the harmful effects of TCPMOH. With new environmental contaminants continually being discovered, the network model developed may be applied to determine the morphological damage any new toxicant may have.

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CP14

Determining Influential Parameters in Nonsmooth Models of Riots

The spread of rioting can be modeled as a sort of social contagion using nonsmooth ODEs, with nonsmoothness arising when a tipping point threshold is crossed, marking an outburst of social activity with a bandwagon-like effect. We are interested in investigating parametric sensitivities of such rioting activity, but the presence of nonsmoothness invalidates classical sensitivity theory. However, thanks to a recent advancement in generalized derivatives theory called lexicographic directional differentiation, nonsmooth modeling frameworks now possess a computationally-relevant theory capable of characterizing local sensitivity information. In this talk, we highlight the nonsmooth sensitivity theory and apply it to a multisite model of the 2005 French riots around Paris, which was validated against a comprehensive data set of police reports. After discovering key parameters driving the rioting activity, we consider other possible scenarios in a non-local sensitivity analysis of this social contagion.

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CP15

Assessing Building Damage After Natural Disasters with Interpretable Convolutional Neural Networks

Natural disasters ravage the world's cities and shores on a monthly basis. Having precise and efficient mechanisms for assessing infrastructure damage is essential to channel resources and minimize the loss of life. Using a dataset that includes labeled pre- and post- disaster satellite imagery, the xBD dataset, we train multiple convolutional neural networks to assess building damage on a per-building basis. In order to investigate how to best classify building damage, we present a highly interpretable deep-learning methodology that seeks to explicitly convey the most useful information required to train an accurate classification model. We also delve into which loss functions best optimize these models. Our findings include that ordinal-cross entropy loss is the most optimal loss function to use and that including the type of disaster that caused the damage in combination with a pre- and post-disaster image best predicts the level of damage caused. The highest accuracy percentage on the testing set that we achieve is 74.6%; the non-optimal nature of this is largely attributed to the limited discernibility between the major and minor damage categories. We also make progress in the realm of qualitative representations of which parts of the images that the model is using to predict damage levels, through gradient class-activation maps. Our research seeks to computationally contribute to aiding in this ongoing and growing humanitarian crisis, heightened by climate change.

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CP15

Galerkin Neural Networks: A Framework for Approximating Variational Equations with Error Control

The past decade has seen a surge of interest in applying neural networks to a range of non-standard applications, including the numerical approximation of partial differential equations. We present a new neural network framework for approximating variational problems based on the traditional Galerkin method. This approach is based on the adaptive construction of a sequence of finite-dimensional subspaces whose basis functions are realizations of a sequence of neural networks. The finite-dimensional subspaces are then used to define a standard Galerkin approximation of the variational equation. We present basic theoretical results regarding the convergence of the method and several examples demonstrating the efficacy of the approach.

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CP15

Data Driven Machine Learning Models For Flood Prediction on the Mississippi River Basin

Floods are one of the most destructive natural disasters but can be highly chaotic and complex to model. Accurate flood prediction models can be critical to minimizing the impact of these events on infrastructure and on the lives of those who live near a floodplain. Traditional, coupled models tend to be computationally expensive due to the considerable amount of data that reflect both spatial and temporal variations of key hydrological components to floods. This presentation will demonstrate an approach to build hydrological models that can accurately and precisely map river discharge as a function of climate and other geological conditions at a given point in the future. These models will be built using historical data obtained from the Copernicus Satellite.

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CP15

Immune Cell Subset Metacluster Frequencies Across Batches of Cov2-Stimulated Blood Samples

over Time, and in Association with Clinical Metadata

It's not true I never metacluster I didn't like. We're using clustering algorithms on 20-dimensional snapshots of immune cells at a batch level, for many batches, initially "overclustering." We then "metacluster" the z-scored cetroids of the initial clusters, to arrive of cohort-level metacluster classification of diverse T and B cell subsets. Hence we're clustering together thousands to tens of thousands of CD4 and CD T cells per participant, per blood draw, per COV-2 peptide pool stimulation, with 16 participant visits per batch, 5 stimulations per participant visit, and 25 batches and counting. We are using these frequencies as serological measures and to examine as correlates of clinical outcomes.

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CP15

Investigating Fluid Drainage from the Edge of a Porous Reservoir using Physics Informed Neural Networks

Physics Informed Neural Networks (PINNs) is a state-of-the-art tool for finding data-driven solutions to PDEs and discovering parameters in a PDE from a given data. In the present work, we have studied both, in the context of fluid drainage from the edge of a porous reservoir. To the best of our knowledge, this is the first implementation of deep neural networks to study this geophysical phenomenon. In the first part, we investigated the steady-state PDE, called Dupuit-Boussinesq approximation, from both synthetic and experimental data for a range of given input flow values, where training data is provided for the state variable; the water table height. We found that the experimental data displayed features that are not captured by the simple PDE. We also tried to estimate the hydraulic conductivity from both synthetic and experimental data. Furthermore, we solved the estimation problem for the transient flow PDE, using numerical solutions from finite-difference simulations as the input data to infer both the hydraulic conductivity and the outflow boundary condition. We found that the PINNs were able to infer the model parameters with reasonable accuracy, and more importantly, PDE solutions produced by the estimated parameter values were a good fit for the data. Finally, we highlight some of the difficulties in implementing PINNs for studying this problem, for example, when the data does not perfectly match the PDEs or scaling of the misfit terms.

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CP16

Towards a Generalization of Optimization Methods on Manifolds via Diffeological Spaces

In the 1980s, J.M. Souriau introduced firstly diffeological spaces which are a natural generalization of smooth manifolds. However, optimization techniques are only known on manifolds so far. A generalization of these techniques to diffeological spaces is very challenging due to several reasons. For example, there are various definitions of tangent spaces which do not coincide. In addition, one needs to generalize a Riemannian space in order to define gradients which are necessary for optimization methods. In this talk, we present a suitable definition of a tangent space in view to optimization methods. Based on this definition, we define a diffeological Riemannian space and a diffeological gradient. In order to update the iterates in an optimization algorithm on diffeological spaces, we present a diffeological retraction and the Levi-Civita connection on diffeological spaces.

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CP16

On Parametric Second-Order Conic Optimization

We study the parametric analysis of a second-order conic optimization problem, where the objective function is perturbed along a fixed direction. We introduce the notions of nonlinearity interval and transition point which serve as stability regions of the optimal partition. Finally, under some regularity conditions, we propose numerical procedures to compute a nonlinearity interval or to identify a transition point.

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CP16

Adaptive Optimization of District Heating Network Operation

We propose an adaptive optimization algorithm for operating district heating networks in a stationary regime. The behavior of hot water flow in the pipe network is modeled using the incompressible Euler equations and a suitable energy equation. The algorithm is based on a hierarchy of this system of differential equations to adaptively model physics in the individual pipes of the network depending on the actual state of physics. A posteriori error estimators are used for switching between the models in the hierarchy and to control the discretization of the differential equations. We prove convergence of the adaptive method and present some numerical results that illustrate the applicability of the approach.

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CP17

Improving the Applicability and Efficiency of Monte Carlo Linear Algebra Algorithms

When dealing with large, linear-algebra problems, classical linear-algebra tools are no longer practical because the computational cost is not feasible. The computational cost of well known algorithms are usually $O(N^3)$ for dense matrices, and even linear iterative methods for sparse matrices are not applicable when N is huge. In this case, a Monte Carlo algorithm is the only method that we can actually apply to solve those problems. However, it is not always guaranteed that a Monte Carlo algorithm is convergent and efficient. An appropriate preconditioner and transition probability need to be chosen to make the algorithm reliable. We are interested in seeking the lowest eigenvalue of large matrices. We transform the eigenvalue problem to a scalar equation using the Shur complement, and this scalar equation includes the inverse of the matrix, which can be obtained by solving a system of linear equations. Our goal is to find the appropriate preconditioner to reduce the sample variance when solving a linear system by a Monte Carlo algorithm. We suggest to sample a tile of a matrix, instead of one element at a time. We show that tiling reduces the variance for when we have a dense random matrix as a coefficient matrix.

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CP17

On the Classification Capabilities of Topological Data Analysis

Topological Data Analysis (TDA) has been applied to enhance Machine Learning (ML) pipelines across different application domains. TDA has been widely used to provide topological interpretations of data in topological descriptors to allow ML tasks such as clustering or supervised classification. Multiscale relationships between data are discovered and processed during filtered simplicial complexes construction and persistence computation, but once desired topological features are computed, all those relationships are discarded. However, taking advantage of both the TDA results and the entire topological invariants discovering process would help address current classification challenges. This work aims to present preliminary results on TDA's direct application to supervised learning with no further ML stage. A label propagation algorithm on filtered simplicial complexes based on Link and Star operators will be presented. The main idea is to select a sub-complex from the filtration and perform a labeling propagation process based on the simplex's Link to classify. In this method, the label of maximal contribution is used to label an unlabeled simplex. Filtration values are used in the labeling process as tie disambiguation. The proposed algorithm is applied to imbalanced data classification and mislabeled-data identification, correction, and classification. Finally, experimental results will be presented by comparing the proposed algorithm with other neighbor-based classifiers.

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CP17

Marginal Posteriors with Truncated Marginal Ratio Estimation

In physics and astronomy, marginal posteriors play a pivotal role in constraining the parameters of probabilistic models. Typically these are nonlinear functions of many random variables called simulators. In standard practice, inference algorithms estimate the posterior of all stochastic variables jointly before marginalization. For complex simulators this approach can be intractable. We present truncated marginal ratio estimation: an algorithm that efficiently estimates any marginal posterior by constraining analysis to plausible regions of parameter space through an iterative scheme. It is based on amortized likelihood-to-evidence ratio estimation using a trained binary classifier and differs from existing sequential approaches. It enables: (a) automatic reuse of the simulations for hyper-efficient follow-up studies of alternative observations, (b) efficient coverage tests of the estimated marginal posteriors, and (c) marginal inference of high-dimensional complex posteriors. Since it is a likelihood-free, or simulation-based, method it is applicable when the likelihood is only implicitly defined, i.e. when it is possible to sample the likelihood but not evaluate it. We show that our method can require at least an order of magnitude fewer simulations on typical use-cases than likelihood-based approximate inference. We offer a functional prototype open-source package swyft at https://github.com/undark-lab/swyft.

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CP17

Analyzing the Infection Risk of Healthcare Workers for Covid-19 with a New Adaptive Bayesian Lasso Exponential Random Graph Model

In this paper, we propose an Adaptive Bayesian Lasso Exponential Random Graph Model. This model allows the posterior distribution for each parameter to have an individualized variance. The Gibbs Sampling algorithm is derived, and we apply this new flexible model to analyze the infection risk of healthcare workers for COVID-19. Our results show an improvement to the traditional Bayesian Exponential Random Graph model which is significant in light of the promising applications of this newly proposed method.

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CP17

A Neural Network Ensemble Approach to System Identification

We present a new algorithm for learning unknown governing equations from trajectory data, using neural networks. Given samples of solutions $x(t)$ to an unknown dynamical system $\dot{x}(t) = f(t, x(t))$, we approximate the function f using an ensemble of neural networks. We express the equation in integral form and use Euler method to predict the solution at every successive time step using at each iteration a different neural network as a prior for f. This procedure yields N-1 time-independent networks, where N is the number of time steps at which $x(t)$ is observed. Finally, we obtain a single approximation of the function $f(t, x(t))$ by neural network interpolation. Unlike our earlier work, where we numerically computed the derivatives of data, and used them as target in a Lipschitz regularized neural network to approximate f, our new method avoids numerical differentiations, which are unstable in presence of noise. We test the new algorithm on multiple examples, such as the Lotka-Volterra system and the Damped Pendulum equation both with and without noise in the data. We empirically show that generalization and recovery of the governing equation improve by adding a Lipschitz regularization term in our loss function and that this method improves our previous one especially in presence of noise, when numerical differentiation provides low quality target data. Finally, we compare our results with the method proposed by Raissi, et al. arXiv:1801.01236 (2018).

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CP17

Large Deviation Principle for Local Empirical Measure of Coulomb Gases at Intermediate Temperature Regime

We work with Coulomb gases at an intermediate temperature regime. We define a local empirical field and identify a critical temperature scaling. We show that if the scaling of the temperature is supercritical, the local empirical field satisfies an LDP with an entropy-based rate function. We also show that if the scaling of the temperature is subcritical, the local empirical field satisfies an LDP with an energy-based rate function. An important idea in this work is to exploit the different scaling relations satisfied by the Coulomb energy and the entropy.

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CP18

Critical Thresholds in a Nonlocal Euler System with Relaxation

We propose and study a nonlocal Euler system with relaxation, which tends to a strictly hyperbolic system under the hyperbolic scaling limit. We will derive a precise critical threshold for this system in one dimensional setting. Our result reveals that such nonlocal system admits global smooth solutions for a large class of initial data. Thus, the nonlocal velocity regularizes the generic finite-time breakdown in the pressureless Euler system. We will also look into a one-dimensional 2×2 hyperbolic Eulerian system with local relaxation from critical threshold perspective. The system features dynamic transition between strictly and weakly hyperbolic.

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CP18

A Superconvergent Hybrid Method of Spectral Elements and Generalized Weighted Residuals on Irregular Domains

Spectral element methods, such as those using tensor-product Gauss-Lobatto points, are well known to superconverge over regular domains. However, superconvergence is often lost on irregular domains due to distorted elements. We introduce a novel hybrid method, which uses a Schwarz alternating process to combine superconvergent spectral elements with Gauss-Lobatto points in the interior of the domain with a method of generalized weighted residuals (GWR) near the boundary. Specifically, we use a GWR formulation called the extended adaptive stencil finite element method (AES-FEM), which overcomes element-quality dependence of Lagrange finite elements. Our resulting hy-

brid method, called SPEAF, preserves the global superconvergence of spectral elements, while being able to accommodate irregular domains by using hybrid meshes. We present numerical results in solving parabolic PDEs in 2D and 3D and demonstrate the $\mathcal{O}(h^{p+2})$ convergence rate in ℓ^2 norm and $\mathcal{O}(h^{p+1})$ in H^1 norm with even-degree-p spectral elements in the interior. These superconvergence results match those of spectral elements and exceed those of equidistant finite elements by one order, while approximately preserving their efficiency. We describe the simplified mesh-generation process of SPEAF with a sublinear time complexity, and compare the accuracy and efficiency of SPEAF with standard Lagrange finite elements and spectral elements.

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CP18

Iterative High Order Numerical Method for Multiple Scattering

This paper outlines a new iterative method for determining the scattered wave for two dimensional multiple acoustic scattering problems. We seek to approximate the total wave as it is scattered off of multiple arbitrarily shaped obstacles. This is done by enclosing each obstacle in a circular artificial boundary and generating a curvilinear coordinate system for the computational region between the obstacles and the artificial boundary. We treat each obstacle as a separate singular acoustic scattering problem and use a finite difference method to create a linear system whose solution will approximate the scattered wave. The forcing vector in the linear system is determined from the total influence on the obstacle boundary from the incident wave and the scattered waves from the other obstacles. In each iteration, we solve the singular acoustic scattering problem for each obstacle by using the scattered wave approximations from the other obstacles obtained from the previous iteration. The iterations continue until the solutions converge. I will include numerical results which demonstrate the accuracy and advantages of our technique.

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CP18

Parameter Identification in Three-Dimensional Electrostatics for Magnetohydrodynamics

Magnetohydrodynamics (MHD) is the study of a charged medium flowing through a magnetic field. For this talk, the working fluid is assumed to be a steady state singularly ionized plasma moving uniformly down the channel. Similarly, the magnetic field is assumed to be a steady state applied field, neglecting the induced field. Introducing the ion-slip term into the generalized Ohm's law, and coupling Maxwell's equations results in a non-linear system of PDE's whose solution is the electric field and current, **E** and **J** respectively. Using a matrix representation of the cross-product, an explicit form of Ohm's law is presented. Well-posedness of both the forward problem and the inverse problem, with a parameter set consisting of the fluid flow, conductivity, applied magnetic field, hall parameter, and ion-slip parameter is presented. Numerical validation of the parameter estimation will also be discussed, utilizing COMSOL to apply FMGRES and finite element techniques to complex geometry, with electrodes and loads being included in the model. Both the continuous and segmented Faraday configurations will be explored.

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CP18

Interaction of Optical Pulses in Nonlinear Media

Interaction of optical pulses in Nonlinear optical media is studied numerically and analytically. The pulse dynamics are simulated by wave propagation techniques. The numerical simulations agree with the results of the analytical model. The new results explain the interaction of pulses at the interface and provide conditions for reflection or transmission. This provides an opportunity to analyze the interaction in different types of media including diffusive nonlinear media.

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CP18

A Feynman-Kac Based Numerical Method for Solving Local and Non-Local Transport Problems

The exit time probability, which gives the likelihood that a particle leaves a prescribed region in the phase space of a dynamical system at, or before, a given time, is arguably one of the most natural and important transport problems. Here we present an accurate and efficient numerical method for computing this probability for systems described by nonautonomous (time-dependent) stochastic differential equations (SDEs) and their equivalent Fokker-Planck partial differential equations. The method is based on the direct approximation of the Feynman-Kac formula that establishes a link between the adjoint Fokker- Planck equation and the forward SDE. The method is unconditionally stable, exhibits second-order convergence in space, first-order convergence in time, and, it is straightforward to parallelize. In the local transport case, the SDEs are driven by Brownian motion, and in the nonlocal case, by a combination of Brownian motion and Poisson jump processes describing nonlocality with a finite horizon kernel in the corresponding partial integrodifferential equation (PIDEs). As a natural extension of boundary conditions for local PDEs, we consider volume constraints in the nonlocal case. Applications of the proposed method to local transport include advection-diffusion of passive tracers in fluid flows exhibiting chaotic advection and runaway acceleration of electrons in a plasma.

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CP19

Dory: Overcoming Barriers to Computing Persistent Homology

Persistent homology (PH) is a tool in topological data analysis (TDA) that computes multi-scale topologically invariant properties of high-dimensional data that are robust to noise. While PH has revealed useful patterns across various applications, computational requirements have been limited to small data sets of a few thousand points. We present Dory, an efficient and scalable algorithm that enables the computation of persistent homology to large data sets. Dory uses significantly less memory and computation time when compared to the best of the published algorithms, and scales to process data sets with millions of points. As an application, we compute PH of the human genome at the high resolution of 1 kilobase from a genome-wide Hi-C data set. Results show that the topology of the human genome changes significantly upon treatment with auxin, a chemical that degrades cohesin, corroborating the hypothesis that cohesin plays a crucial role in loop formation in DNA.

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CP19

The Shape of Things to Come: Topological Data Analysis and Plant Biology

Shape is foundational to biology. Observing and documenting shape has fueled biological understanding as the shape of biomolecules, cells, tissues, and organisms arise from the effects of genetics, development, and the environment. The vision of topological data analysis (TDA), that data is shape and shape is data, will be relevant as biology transitions into a data-driven era where meaningful interpretation of large datasets is a limiting factor. We focus first on quantifying the morphology of X-ray CT scans of barley spikes and seeds using topological descriptors based on the Euler characteristic transform. We then successfully train a support vector machine to distinguish and classify 28 different varieties of barley based solely on the 3D shape of their grains. This shape characterization will allow us later to link genotype with phenotype, furthering our understanding on how the physical shape is genetically specified in DNA.

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CP19

A Metric on Directed Graphs and Markov Chains Based on Hitting Probabilities

The shortest-path, commute time, and diffusion distances on undirected graphs have been widely employed in applications such as dimensionality reduction, link prediction, and trip planning. Increasingly, there is interest in using asymmetric structure of data derived from Markov chains and directed graphs, but few metrics are specifically adapted to this task. We introduce a metric on the state space of any ergodic, finite-state, time-homogeneous Markov chain and, in particular, on any Markov chain derived from a directed graph. Our construction is based on hitting probabilities, with nearness in the metric space related to the transfer of random walkers from one node to another at stationarity. Notably, our metric is insensitive to shortest and average walk distances, thus giving new information compared to existing metrics. We use possible degeneracies in the metric to develop an interesting structural theory of directed graphs and explore a related quotienting procedure. Our metric can be computed in $O(n^3)$ time, where n is the number of states, and in examples we scale up to $n = 10,000$ nodes and $\approx 38M$ edges on a desktop computer. In several examples, we explore the nature of the metric, compare it to alternative methods, and demonstrate its utility for weak recovery of community structure in dense graphs, visualization, structure recovering, dynamics exploration, and multiscale cluster detection.

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CP19

Utilizing the Structure of the Curvelet Transform in Compressed Sensing

Compressed sensing (CS) has empowered quality image reconstruction with fewer data samples than previously thought were required. CS is made possible by a system matrix that satisfies some condition where it is close to invertible, such as the Restricted Isometry Principle in Levels. Much of the theory of compressed sensing applies to a general matrix of this type. The Discrete Curvelet Transform (DCT) has been shown to represent images with a low number of significant coefficients. When combined with a Fourier sensing application, e.g. MRI, the DCT is an effective sparsifying transform. In this work, we consider the specific structure of the DCT. We show that the DCT suggests that the sampling pattern should include a fully sampled region of a specific size, corresponding to the resolution of the coarse filter embedded in the DCT, in the center of the Fourier domain. We take advantage of the structure of the DCT and identify an affine transformation that increases the sparsity of the result. After inclusion of this affine transformation, we modify the resulting optimization problem to comply with the usual form of the problem solved in CS. Remarkably, the system matrix of the resulting problem is the same as the original, which maintains the theoretical guarantees of CS. Because of the increased sparsity, the problem yields images of higher quality for the same number of samples. We present results with data from magnetic resonance and optical images.

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CP19

Robust Cyber-Risk Estimation in IoT Devices

Weak security practices often expose increasingly pervasive IoT systems to (major) cyber-attacks. Third-party cyber-risk management (CRM) solutions are thriving in mitigating such attacks' negative impacts on civilian sectors or else. The pre-requisite to scale the markets for such solutions is robust cyber-risk estimation for IoT systems - both, for individual IoT gadgets, and, for the network formed by such gadgets. We address the problem for individual IoT gadgets that comprise multiple components "stitched" together, each supporting a salient functionality, and often manufactured by heterogeneous vendors. Specifically, we account for the statistical dependencies between the performance measures of (i) different components at a given time, and (ii) the same component over time, to robustly estimate the standard time-dependent Conditional Value at Risk (CVaR) for such gadgets. We exhibit an experimental increase in CVaR-estimation accuracy of up to 90% compared to estimates not considering statistical dependencies. We also derive a mathematical concentration bound of the CVaR metric for a multi-component IoT gadget. Finally, we showcase a rigorous and computationally efficient Bayesian CVaR prediction method that accurately predicts components' future performance. Apart from a clear advantage to the CRM industry, our method is of particular social importance in life-critical IoT gadget settings such as pacemakers and artificial kidneys under resource-drainage (RD) attacks.

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CP19

Emd with Shape-Preserving Spline Interpolation

Empirical mode decomposition (EMD) is a popular, novel, user-friendly algorithm to decompose a given signal into its constituting components, utilizing spline interpolation. In this paper, we equip EMD with a shape-preserving interpolation scheme based on quadratic B-splines. Using numerical experiments, we show that our scheme, which we coin Geometric EMD, or GEMD, outperforms the original EMD, both qualitatively and quantitatively.

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MS1

Robust Monitoring of the Human Head by Electrical Impedance Tomography

This project focuses on applying EIT to head imaging without accurate information on the electrode positions or the shape of the studied patient's head. In medical applications of EIT, the exact shape of the imaged object is usually unknown; even if one has some generic information about the average shape of the imaged part of the human body, the natural variations between different subjects are often significant and EIT is known to be extremely sensitive to geometric mismodelling. In this talk I will present two different methods for handling the problem on a computational FEM head model. On the one hand, I will show results with machine learning approaches, such as support vector machine (SVM) and neural networks (NN), used to binary classify the type of stroke occurred, hemorrhagic or ischemic. Albeit really fast, this method wont provide a full image reconstruction. On the other hand, we apply the approximation error approach, where the error caused by the mismodeling is included as an extra additive noise process in the measurement model, its statistics are estimated in advance based on heavy simulations and prior knowledge on all unknown parameters, and finally the actual inversion is performed within the Bayesian paradigm. These are joint works with M. Santacesaria, N. Hyvönen, J. Kaipio and V. Kolehmainen.

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MS1

Graph U-Net for 2D Electrical Impedance Tomography

The most comprehensive forward model for electrical impedance tomography requires discretizing the domain, often into a finite element method (FEM) mesh. The inverse problem, often referred to as EIT reconstruction, also typically takes place with the conductivity distribution defined over a FEM mesh. Previously, neural networks have been incorporated into reconstruction methods with the use of fully connected layers or by restricting discretization to Euclidean grids in order use traditional convolutional layers. Recently, outside of EIT, graph convolutional networks (GCNs) have grown in popularity because they share many of the same benefits as traditional convolutional networks except that they are flexible enough to operate over graph data. In this work, a GCN with a U-net architecture is used to post process recovered conductivity distributions defined over a FEM mesh, leading to increased sharpness and reliability in the final reconstruction. The GCN is trained using simulated data and preliminary results are provided for experimental ACT3 and KIT 4 data sets.

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MS1

Direct 3D Electrical Impedance Tomography Reconstructions from Simulated Electrode Data

Until recently, most Complex Geometrical Optics (CGO)-based reconstruction methods have focused on 2D image reconstruction. 3D CGO-based methods have primarily focused on theoretical studies and assume continuum data on the entire boundary of the domain. This work is the first to adapt the 3-D $\mathbf{t}^{\mathbf{exp}}$ method to cases with simulated electrode data and the first to implement a 3-D Calderón method on a sphere with simulated electrode data. Results for the 3D CGO-based methods are comparable to their 2D counterparts. In addition, these methods are compared to more common regularized non-linear least squares methods. The effect of number of electrodes and noise level are investigated across all methods. Extending on the work with spherical domains, we present 3D CGO-based reconstructions in ellipsoidal domains with simulated electrode data. To improve the image quality, we introduce deep learning post-processing of these 3D images.

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MS1

Combining Real World Measurements of EIT with Neural Networks for Stroke Classification

Electrical Impedance Tomography (EIT) is an emerging non-invasive medical imaging modality. It is based on the measurements of boundary electrical currents and voltages, leading to recovering the internal conductivity distribution. The mathematical task of EIT image reconstruction is a nonlinear and ill-posed inverse problem, typically resulting in blurred images. One promising application is stroke-EIT, or classification of stroke into either ischemic or hemorrhagic. Ischemic stroke involves a blood clot, preventing blood flow to a part of the brain causing a low-conductivity region. Hemorrhagic stroke means bleeding in the brain causing a high-conductivity region. In both cases the symptoms are identical, so a cost-effective and portable classification device is needed. Typical EIT images are not optimal for stroke-EIT because of blurriness. In this talk we first approximate the idealized boundary condition, that is Dirichlet-to-Neumann(DN) map, from the practical boundary electrode measurements of Complete Electrode Model (CEM). We then use the idealized DN map to extract robust features called Virtual Hybrid Edge Detection (VHED) functions that have a geometric interpretation and whose computation from EIT data does not involve calculating a full image of the conductivity. We report the measures of accuracy for the stroke prediction using VHED functions on data sets that differ from the training data used for the training of neural network.

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MS2

Integrable Dynamics of Curves in the Pseudoconformal 3-Sphere

We consider evolution equations for curves in the 3-dimensional sphere that are invariant under the group $SU(2,1)$ of pseudoconformal transformations, which preserves the standard contact structure on the sphere. In particular, we investigate how invariant evolutions of Legendrian and transverse curves induce both new and well-known integrable systems and hierarchies at the level of their geometric invariants.

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MS2

High-Order Rogue Waves and Solitons, and Solutions Interpolating Between Them

A family of exact solutions to the focusing nonlinear Schrdinger equation is presented that contains fundamental rogue waves and multiple-pole solitons of all orders. The family is indexed with a continuous parameter representing the "order" that allows one to continuously tune between rogue waves and solitons of different integer orders. In this scheme, solitons and rogue waves of increasing integer orders alternate as the continuous order parameter increases. For example, the Peregrine solution can be viewed as a soliton of order three-halves. We show that solutions in this family exhibit certain universal features in the limit of high (continuous) order.

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MS2

Instability of Breathers and Double-Periodic Waves in the Focusing NLS Equation

I will discuss precise analytical results on linear instability of Akhmediev breathers, Kuznetsov-Ma breathers, and Peregrine's rogue wave. These solutions are degenerate cases of the double-periodic solutions to the cubic NLS (nonlinear Schrodinger) equation. The wave function modulus of the double-periodic solutions is periodic both in space and time coordinates; such solutions generalize the standing waves which have the time-independent and space-periodic wave function modulus. Similar to breathers and standing waves, the double-periodic solutions are spectrally unstable and this instability is related to the bands of the Lax spectrum outside the imaginary axis.

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MS2

On Spectral Theory of Soliton and Breather Gases

for Integrable Systems

Solitons and breathers are localized solutions of integrable systems that can be viewed as particles of complex statistical objects called soliton and breather gases. In this talk we briefly review some main equations of the spectral theory of soliton gases for integrable systems and discuss rigorous analysis of these equations.

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MS3

The Impact of Changing Behavior, Sentiments, and Risk Perception on Covid-19 Transmission

COVID-19 is a respiratory disease caused by coronavirus, SARSCOV2. The disease has led to over 81 million cases, and with over 2 million deaths worldwide. In the current social and political climate, the risk of COVID-19 infection is driven by peoples perception of risk of the infection. A number of factors drive public perception of disease risk, these include peoples beliefs, knowledge, and information about a disease. In this seminar, I present two different models for COVID-19 looking at peoples behavior and their sentiments about the disease. One model uses game theory and appropriate payoff functions relating to the perception of risk measured using disease incidence and severity of infection to account for a series of human behaviors. Which leads to a complex interplay between the epidemiological model, that affects success of different strategies, and the game theoretic behavioral model, which in turn affects the spread of the disease. The second model uses tweets from twitter to account for peoples sentiments about the disease. It also takes into account negative sentiments driven by misinformation. The results from these models shows that rational behavior of susceptible individuals can lead to a second wave of the pandemic. To reduce the burden of the disease in the community, it is necessary to ensure positive sentiments and feelings and to incentivize such altruistic behavior by infected individuals as voluntary self-isolation.

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MS3

Optimal Control Applied to Models of Invasive Species in Rivers

Using a parabolic PDE model representing an invasive population in a river, we investigate controlling the water discharge rate as a management strategy. Our goal is to use the control to keep the invasive population downstream. Using an optimality system, consisting of our population PDE, an adjoint PDE, and corresponding optimal control characterization, we illustrate some numerical simulations to show how far upstream the invasive population reaches.

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MS3

Estimation of Partial Differential Equations

In many physical applications, the system's state varies with spatial variables as well as time. Such systems are modelled by partial differential equations and the state evolves on an infinite-dimensional space. Systems modelled by delay-differential equations are also infinite-dimensional systems. The full state of these systems cannot be measured. Observer design is an important tool for estimating the state from available measurements. The idea is to combine information from measurements and the model, both of which contain errors, to arrive at a estimate of the system state. Often only some aspect of the state needs to be estimated, not the whole state. This, and also the nature of disturbances, should guide the choice of observer design. The well-known Kalman filter is described, and also several other types of estimators for output estimation of linear infinite-dimensional systems. Another factor in estimator accuracy for systems with spatial dependence is the location of the sensors. A practical framework for constructing finite-dimensional estimators that provide performance arbitrarily close to optimal is described. Some results are described and illustrated with computational results.

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MS3

Consensus and Control of Opinion Formation Models

We analyze the asymptotic behavior of a Hegselmann-Krause opinion formation model with time delay. Under appropriate assumptions, we prove exponential consensus estimates when the time delay satisfies a suitable smallness assumption. Our arguments are based on a Lyapunov functional approach and require careful estimates on the trajectories. We then study the mean-field limit from the many-individual Hegselmann-Krause equation to the continuity-type partial differential equation as the number of individuals goes to infinity. For the limiting equation, we prove global-in-time existence and uniqueness of measure-valued solutions. We also use the fact that constants appearing in the consensus estimates for the particle system are independent of the number of individual to extend the exponential consensus result to the continuum model. Some related control problems are also illustrated.

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MS4

Non-Asymptotic Estimation of Risk Measures using Stochastic Gradient Langevin Dynamics

In this talk we will discuss the approximation of arbitrary law invariant risk measures. The approximation algorithm we propose is based on stochastic gradient Langevin dynamics, which can be seen as a version of the stochastic gradient descent used in various learning problems. We will present both theoretical, non-asymptotic convergence rates of the approximation algorithm and numerical simulations. We will particularly discuss the case of the average value-at-risk.

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MS4

Portfolio Optimisation within a Wasserstein Ball

We study the problem of active portfolio management where an investor aims to outperform a benchmark strategy's risk profile while not deviating too far from it. Specifically, an investor considers alternative strategies whose terminal wealth lie within a Wasserstein ball surrounding a benchmark's – being distributionally close – and that have a specified dependence/copula – tying state-by-state outcomes – to it. The investor then chooses the alternative strategy that minimises a distortion risk measure of terminal wealth. In a general (complete) market model, we prove that an optimal dynamic strategy exists and provide its characterisation through the notion of isotonic projections. We further propose a simulation approach to calculate the optimal strategy's terminal wealth, making our approach applicable to a wide range of market models. Finally, we illustrate how investors with different copula and risk preferences invest and improve upon the benchmark using the Tail Value-at-Risk, inverse S-shaped, and lower- and upper-tail distortion risk measures as examples. We find that investors' optimal terminal wealth distribution has larger probability masses in regions that reduce their risk measure relative to the benchmark while preserving the benchmark's structure.

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MS5

Fast Computation of Little Interpolants

A fundamental point in the implementation of local high-dimensional interpolants is the construction of fast partitioning and searching routines, which allow us to efficiently organize the set of data points. This request derives from the need of detecting suitable subsets useful to construct the local interpolant. In particular, in the 2d and 3d settings the computation of Little interpolants needs configurations of triangles or tetrahedra whose vertices are given by the interpolation nodes. It is therefore important for each point to find the nearest neighbors so as to efficiently compute the interpolant. Here we present the use of a fast searching procedure based on the partitioning of the domain and of the scattered data set in squares or cubic blocks. Several numerical results will be presented to show the efficiency of the proposed algorithms.

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MS5

Inverse Distance Weighting-Partition of Unity Methods: An Overview

In this introductive talk we give a review of some recent published results on Inverse Distance Weighting-Partition of Unity Methods.

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MS5

Solving Poisson Equation with Dirichlet Conditions Through Multinode Shepard's Operators

The multinode Shepard operator is a linear combination of local polynomial interpolants with inverse distance weighting basis functions. This operator can be rewritten as a blend of function values with cardinal basis functions, which are a combination of the inverse distance weighting basis functions with multivariate Lagrange fundamental polynomials. The key for simply computing the latter, on a unisolvent set of points, is to use a translation of the canonical polynomial basis and the $PA = LU$ factorization of the associated Vandermonde matrix. In this talk, we propose a method to numerically solve a Poisson equation with Dirichlet conditions through multinode Shepard interpolants by collocation. This collocation method gives rise to a collocation matrix with many zero entrances and a smaller condition number with respect to the one of the well known Kansa method. Numerical experiments show the accuracy and the performance of the proposed collocation method.

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MS5

Multivariate Fekete-Like Interpolation and Differentiation on Scattered Data

Interpolation of functions by polynomials is one of the basic parts of Approximation Theory. The usual representation of the interpolation polynomials is given through the Lagrange fundamental polynomials, which are expressed, in the standard form, in terms of the Vandermonde determinants. From the computational point of view, determinants can be difficult to handle and are known to be highly unstable. In this talk, we propose a simple procedure for numerically computing the Lagrange interpolation polynomial of total degree on a unisolvent set of points in $\mathbb{R}^s$. We suggest the use of the canonical polynomial basis centered at a fixed point $\overline{\mathbf{x}} \in \mathbb{R}^s$ and the $PA = LU$ factorization for solving the associated Vandermonde system to compute the coefficients of the Taylor polynomial. We use these coefficients to estimate function and derivative values of a function in multivariate polynomial interpolation and we present error bounds providing information about the geometry of the nodes which guarantees good accuracy of approximation. Finally, we numerically test the accuracy of approximation of the proposed method by choosing a subset of Fekete points in a set of Halton points using a fast algorithm [Sommariva, A., Vianello, M. (2009). Computing approximate Fekete points by QR factorizations of Vandermonde matrices. Computers & Mathematics with Applications, 57(8), 1324-1336].

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MS6

Price Impact Equilibrium with Transaction Costs and Twap Trading

In this talk, I will discuss an equilibrium model with transaction costs and price impact where two agents are incentivized to trade towards a target. The two types of frictions – price impact and transaction costs – lead the agents to two distinct changes in their optimal investment approach: price impact causes agents to continuously trade in smaller amounts, while transaction costs cause the agents to cease trading before the end of the trading period. As the agents lose wealth because of transaction costs, the exchange makes a profit. I will also discuss the existence of a strictly positive optimal transaction cost from the exchange's perspective.

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MS6

Trading with the Crowd

We formulate and solve a multi-player stochastic differential game between financial agents who seek to cost-efficiently liquidate their position in a risky asset in the presence of jointly aggregated transient price impact, along with taking into account a common general price predicting signal. The unique Nash-equilibrium strategies reveal how each agents liquidation policy adjusts the predictive trading signal to the aggregated transient price impact induced by all other agents. This unfolds a quantitative relation between trading signals and the order flow in crowded markets. We also formulate and solve the corresponding mean field game in the limit of infinitely many agents. We prove that the equilibrium trading speed and the value function of an agent in the finite N-players game converges to the corresponding trading speed and value function in the mean field game at rate $O(N^{-2})$. In addition, we prove that the mean field optimal strategy provides an approximate Nash-equilibrium for the finite-player equilibrium.

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MS6

Excursions in Math Finance

The risk and return profiles of a broad class of dynamic trading strategies may be characterized in terms of excursions of a price process away from a reference level. We propose a mathematical framework for the risk analysis of such strategies, based on a description in terms of price excursions, first in a pathwise setting, without probabilistic assumptions, then in a Markovian setting, using Ito's excursion theory for Markov processes. We introduce the notion of d-excursion, defined as a path that deviates by d from a reference level before returning to this level. We show that every continuous path has a unique decomposition into d-excursions, which is useful for scenario analysis of dynamic trading strategies, leading to simple expressions for the number of trades, realized profit, maximum loss, and drawdown. As d is decreased to zero, properties of this decomposition relate to the local time of the path. When the underlying asset follows a Markov process, we combine these results with Ito's excursion theory to obtain a tractable decomposition of the process as a concatenation of independent d-excursions, whose distribution is described in terms of Ito's excursion measure. Finally, we describe a non-parametric scenario simulation method for generating paths whose excursion properties match those observed in empirical data. Based on joint work with Anna Ananova and Rama Cont.

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MS7

Asymptotic Perturbation of the Boundary of An Elliptic Operator

We study the behavior of the solution to an elliptic equation when a Dirichlet condition is replaced by a Neumann condition (or vice-versa) on a small subset ω_ε of the boundary. This problem originates in part in the optimal design of photonics components. We derive the general structure of the first term in the asymptotic expansion of the solution, in terms of the relevant measure of smallness of ω_ε. We also give explicit examples when the set ω_ε is a surfacic ball in R^d, $d = 2, 3$.

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MS7

A Hybrid Coordinate Transform Method for Electromagnetic Scattering by a Grating

We study a hybrid coordinate-transform method for solving the time-harmonic Maxwell equations in a 2D domain containing a surface-relief grating. We consider a problem where both the permittivity and permeability are orthotropic. One application of this method is modeling thin-film solar cells. We derive an integral equation similar to Rellichs identity and use it to prove the scattering problem has a unique solution as long as non-trapping conditions hold. We discuss convergence results for the hybrid method, and show a numerical example with a sinusoidal grating.

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MS7

Lorentz Resonance in the Homogenization of Plasmonic Crystals

We explain the sharp Lorentz resonances in plasmonic crystals that consist of 2D nano dielectric inclusions as the interaction between resonant material properties and geometric resonances of electrostatic nature. One example of such plasmonic crystals are graphene nanosheets that are periodically arranged within a non-magnetic bulk dielectric. We derive an analytic formula for the Lorentz resonances which decouples the geometric contribution and the frequency dependance. This formula comes rigorously from the corrector equation in the process of homogenization, and it can be used for efficient computation. This is joint work with Robert Lipton and Matthias Maier.

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MS8

Representation of Convex Geometries with Colors, Ellipses and Circles

Convex geometries are the closure systems where the associated closure operator satisfies the anti-exchange axiom. Every finite convex geometry can be embedded into a geometry of point configuration in some n-dimensional Euclidean space, where the closure operator is a convex hull operator. An attempt of generalizing points to balls and finding representations of convex geometries by circles on the plane brought to discovery of an obstruction, the Weak Carousel Property. In Summer 2020 we launched a PolyMath REU project, where we checked all convex geometries on 4 and 5 element sets and discovered 49 that resist representation by circles on the plane. Among those we identified 22 that cannot be represented due to the Triangle or the Opposite Properties. Further generalization to representation by ellipses shows that finding an obstruction in this case turns to be more elusive. We also introduce a new type of representation that involves unary predicates (colors) and investigate its connection with the circle representation.

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MS8

Cospanning Characterizations of Antimatroids and Convex Geometries

Given an operator, say σ, two sets X and Y are *cospanning* if $\sigma(X) = \sigma(Y)$. The corresponding equivalence relation, called cospanning, was investigated for greedoids in much detail (Korte, Lovasz, Schrader; 1991). Moreover, these relations determine greedoids uniquely. In fact, the feasible sets of a greedoid are exactly the inclusion-wise minimal sets of the equivalence classes. In this research, we show that feasible sets of convex geometries are the inclusion-wise maximal sets of the equivalence classes of the corresponding closure operator. Same as greedoids, convex geometries are uniquely defined by the corresponding cospanning relations. For each closure operator σ, an element $x \in X$ is *an extreme point* of X if $x \notin \sigma(X - x)$. The set of extreme points of X is denoted by $ex(X)$. We prove, that if σ has the anti-exchange property, then for every set X its equivalence class $[X]_\sigma$ is the interval $[ex(X), \sigma(X)]$. It results in the one-to-one correspondence between the cospanning partitions of an antimatroid and its complementary convex geometry. In summary, cospanning characterizations of combinatorial structures allow us to obtain new properties of closure operators, extreme point operators and their interconnections.

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MS8

Finding Monarchs for Excluded Minor Classes of Matroids

I will begin by giving a general overview of what it means to find monarchs for excluded minor classes. In a paper that appeared in 2018, I used the Strong Splitter Theorem to give a short proof of Oxley's result that the class of binary matroids with no 4-wheel minor consists of a few small matroids and an infinite family of maximal 3-connected rank

r matroids known as the binary spikes. Such a family is called a monarch for the excluded minor class. This proof essentially comes down to finding the monarchs for non-regular matroids with no minors isomorphic to a 9-element rank 4 matroid known as P_9 or its dual P_9^*. In a paper that appeared this year (Australasian Journal of Combinatorics, 79(3), 302326), I was able to strengthen the result by characterizing the class of binary non-regular matroids with no minor isomorphic to just P_9^*. The only members of this class are the rank 3 and 4 binary projective geometries, a 16-element rank 5 matroid, and two monarchs: the rank r binary spikes with $2r + 1$ elements mentioned earlier and another infinite family with $4r - 5$ elements. As a consequence, a simple binary matroid of rank at least 6 with no P_9^*-minor has size at most $\frac{r(r+1)}{2}$ and this bound is attained by the rank r complete graph. This is one of few excluded minor classes for which the members are so precisely determined.

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MS8

Ehrhart tensor polynomials

An extension of the Ehrhart polynomial to tensor valuations on lattice polytopes is introduced. In particular, we initiate the study of the Ehrhart tensor polynomial, its coefficients, and its coefficients in a certain binomial basis - an extension of the h^*-polynomial. We will concentrate on the matrix case providing comparisons to classical Ehrhart theory. The reciprocity results of Ehrhart and MacDonald are extended, a Pick-type theorem is given, as is a result analogous to Stanley's nonnegativity. This is joint work with Monika Ludwig (TU Wien) and, separately, with Soren Berg (Fit Analytics) and Katharina Jochemko (KTH Stockholm).

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MS9

Modeling Fracture Dissolution in Acid Fracturing Treatments with Viscous Fingering

In acid fracturing treatments, a fracture is firstly created by injecting pad fluid, followed by acid injection. The fracture conductivity is created by non-uniform acid-etching on fracture surfaces, which is usually achieved by applying acid viscous fingering technique where a low-viscosity acid is injected into a high-viscosity pad fluid. To predict fracture conductivity, a detailed description of rough acid-fracture surfaces is required. We modeled fracture dissolution in acid fracturing treatments with acid viscous fingering. The following processes were considered in our model: (1) fluid flow inside fracture, (2) acid and polymer transport, (3) mineral dissolution on fracture surfaces, and (4) the change of fracture geometry. The coupled system was solved numerically based on finite volume methods and fracture geometry was updated using a moving mesh technique. Our simulation results reproduced the non-uniform acid-etching phenomenon observed in experiments. Effects of (1) reservoir mineral heterogeneity, (2) perforation spacing, and (3) alternating injection of pad and acid on fracture dissolution were investigated. We found that viscous fingering creates thin acid-etched channels even the reservoir is relatively homogeneous. The perforation spacing should be large enough to avoid the merging of fingers but not too large to constrain the finger height. Alternating injection of pad and acid suppresses acid washout and prevents acid-fracture from collapsing near wellbore.

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MS9

The Hybrid-Dimensional Darcy's Law: A Novel Discrete Fracture Model for Fracture and Barrier Networks on Non-Conforming Meshes

In this work, we propose a novel discrete fracture model for flow simulation of fractured porous media containing flow blocking barriers on non-conforming meshes. The methodology of the approach is to modify the traditional Darcy's law into the hybrid-dimensional Darcy's law where fractures and barriers are represented by Dirac-δ functions contained in the permeability tensor and resistance tensor, respectively. As a natural extension of the previous discrete fracture model for highly conductive fractures, this model is able to account for the influence of both highly conductive fractures and blocking barriers accurately on non-conforming meshes. The local discontinuous Galerkin (LDG) method is employed to accommodate the form of the hybrid-dimensional Darcy's law and the nature of the pressure/flux discontinuity. The performance of the model is demonstrated by several numerical tests.

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MS9

Second Order in Time Bound-Preserving Implicit Pressure Explicit Concentration Methods for Contaminant Transportation in Porous Media

In this talk, we apply the implicit pressure and explicit concentration (IMPEC) methods for compressible miscible displacements in porous media. The method can yield a much larger time step size compared with the fully explicit method. However, most IMPEC methods are only of first order in time. In this talk, we will discuss how to construct a second order in time IMPEC method. The basic idea is to add the correction stage after each time step. Moreover, we will also construct the bound-preserving technique to preserve the upper and lower bounds of the concentration. Numerical experiments will be given to demonstrate the good performance of the proposed method.

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MS10
On the Mix-Norm for Stokes Flow

We consider the process of mixing by incompressible fluids in complex geometries. In this setting, a passive tracer field is advected (with the possibility of diffusive effects) by a given fluid velocity in the domain. At any given point in time, the degree of mixedness of the scalar field by the fluid motion is measured by the "mix-norm'. In periodic domains the mix-norm has been shown to be equivalent to a negative fractional-index Sobolev norm, motivating our use of such norms in general geometric settings. We discuss ongoing work in several directions for the efficient, high-order accurate computation of these including Padé approximant and volume potential-based methods, with a view towards a PDE-constrained optimization framework for fluid mixing.

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MS10
A Fast Algorithm for Particles in a Stokes Flow under Quasi-2D Confinement

Varies complex systems in nature, such as colloidal suspensions, membranes and electrolytes, can be modeled as particles under Quasi-2D confinement and withElectroHydroDynamics(EHD) interactions. It is important to understand the collective dynamics of such many-body systems. In this talk, we will introduce coarse-grained models for particle-based simulations of such systems, and then describe fast spectral methods combining analytical reduction and efficient numerical techniques based on the Fast Spherical Harmonic and Fast Fourier Transforms and also Chebyshev polynomials, that can compute electrostatic and hydrodynamic interactions in linear time in the number of particles.

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MS10
Simple and Accurate Quadratures for the Stokes Potentials on Periodic Boundaries

Periodic boundary conditions (PBCs) frequently arise in numerical simulations due to the fact that periodic domains share important physical characteristics with unbounded domains (no artificial boundary effects, translation invariant, infinitely extensible) but are easier to implement (simple finite computational domain, no extra conditions at infinity, allow Fourier analysis). In biomedical applications, for example, PBCs are used in the design of microfluidic devices, in the study of drug delivery in blood vessels, and in the separation of healthy and cancerous cells. In this talk, we describe a novel and simple quadrature method that can accurately and robustly discretize the Stokes surface potential operators on smooth periodic geometries in 2D and 3D.

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MS10
Vortex Dynamics Computed Lagrangian Methods

In this work, we compare two Lagrangian methods for computing vortex dynamics: the panel-particle vortex method and the contour dynamics. The former simulates the entire vortex region while the latter tracks the patch boundary. Both methods employ kernel regularization to control the formation of small scales and a parallel treecode to reduce the computational expense. We will show the results of vortex merger and shear instability.

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MS11
Stochastic Learning Approach for Model-Constrained Optimal Design of Experiment

We present a novel stochastic approach to binary optimization for optimal experimental design (OED) for Bayesian inverse problems governed by mathematical models such as partial differential equations. The OED utility function, namely, the regularized optimality criterion, is cast into a stochastic objective function in the form of an expectation over a multivariate Bernoulli distribution. The probabilistic objective is then solved by using a stochastic optimization routine to find an optimal observational policy. Numerical results for a sensor placement problem for parameter identification using a standard advection-diffusion model will be presented.

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MS11
Multibang Regularization for Parameter Identification Problems

This work is concerned with inverse problems where a distributed parameter is known a priori to only take on values from a given discrete set. This property can be promoted in Tikhonov regularization with the aid of a suitable convex but nondifferentiable regularization term. Using the specific properties of the regularization term, it can be shown that convergence actually holds pointwise. Furthermore, the resulting Tikhonov functional can be minimized efficiently using a semi-smooth Newton method. Convergence rates of the method is obtained under condition on measure of active sets. Additionally, total variation is added to promote regularity on the boundary of the reconstructions.

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MS11

An Improved Penalty Algorithm for Mixed-Integer and Pde-Constrained Optimization Problems

Optimal control problems including partial differential equation (PDE) as well as integer constraints merge the combinatorial difficulties of integer programming and the challenges related to large-scale systems resulting from discretized PDEs. The Branch-and-Bound (BnB) framework, a common solution strategy for such problems, finds the global optimum by searching the combinatorial tree provided by the integer constraints in a clever and efficient way. Unfortunately, BnB methods in a large-scale context can be time-infeasible: either the amount of integer constraints may be too overwhelming, or the solution time of a subproblem inside the BnB combined with the amount of subproblems to be solved can be problematic. Thus, this talk investigates penalization strategies that remove the integrality constraint and add a suitable penalty term to the objective function. Inspired from an existing exact penalty (EXP) algorithm, a novel improved penalty algorithm (IPA) is derived. Utilizing the framework of the EXP algorithm to correctly increase the amount of penalization throughout the iteration, the IPA tries to find an iterate that decreases the current objective function value. This is achieved via the combination of a problem-specific perturbation strategy and an Interior-Point method that is tailored towards this penalization context. Based on a standard stationary test problem, the IPA will be compared to the BnB-routine of Cplex and a basic penalty approach.

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MS11

Total Variation Regularization for Integer Control Problems with One-Dimensional Domains

We propose to regularize integer control problems with one-dimensional domains with a total variation term in the objective. This allows us to derive a trust region algorithm, where the trust region subproblem – after discretization – becomes a linear integer problem. The infinite-dimensional setting allows a meaningful definition of local minimizers and first-order optimality conditions can be subsequently derived. Similarly to trust-region methods for nonlinear optimization the iterates converge to points that satisfy first-order optimality conditions. We demonstrate the theoretical findings on a computational example and show why the current analysis and stationarity concepts hinge on the one-dimensional setting and cannot be generalized straightforwardly to higher dimensions.

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MS12

Computing the Quasipotential for Nongradient SDEs

The quasipotential is a crucial function for quantifying transitions between attractors of dynamical systems evolving according to nongradient SDEs with small white noise. It can be viewed as an analogue of the potential function for gradient SDEs in which the invariant density is given by the Gibbs density, the transition rates given by the Kramer's/Langer's formula, and the maximum likelihood transition paths go directly uphill or downhill. Likewise, the quasipotential allows us to approximate the invariant probability measure and find transition rates and maximum likelihood transition paths for nongradient SDEs. Unfortunately, it cannot be found analytically except for special cases. We develop Dijkstra-like numerical methods for computing the quasipotential in whole regions for 2D and 3D SDEs. We test them on a number of examples with point attractors and limit cycles and demonstrate their efficiency and accuracy. We apply them to genetic switch models and to Lorenz'63 with added small white noise for a parameter range embracing the case where the strange attractor and the asymptotically stable equilibria coexist.

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MS12

Graphical Representations of Matern Fields: Theory and Applications

In this talk I will introduce graphical representations of stochastic partial differential equations as a way to approximate Matern Gaussian fields. Approximation error guarantees will be established building on and generalizing the theory of spectral convergence of graph Laplacians. Graphical representations allow inference and sampling with linear algebra methods for sparse matrices, thus reducing the computational cost of Gaussian field approaches. In addition, they bridge and unify several models in Bayesian inverse problems, spatial statistics and graph-based machine learning. We demonstrate through examples in these three disciplines that the unity revealed by graphical representations facilitates the exchange of ideas across them.

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MS12

Convergence of Unadjusted Hamiltonian Monte Carlo for Mean-Field Models

In this talk we consider the unadjusted Hamiltonian Monte Carlo algorithm applied to high-dimensional probability distributions of mean-field type. We evolve dimension-free convergence and discretization error bounds. These bounds require the discretization step to be sufficiently small, but do not require strong convexity of either the unary or pairwise potential terms present in the mean-field model. To handle high dimensionality, we use a particlewise coupling that is contractive in a complementary particlewise metric. This talk is based on joint work with Nawaf Bou-Rabee.

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MS13

Market Efficient Portfolios in a Systemic Economy

We study the ex-ante maximization of market efficiency, defined in terms of minimum deviation of market prices from fundamental values, from a centralized planner's perspective. Prices are pressured from exogenous trading actions of leverage targeting banks, which rebalance their portfolios in response to asset shocks. We develop an explicit expression for the matrix of asset holdings which minimizes market inefficiency, and characterize it in terms of two key statistics: the banks' systemic significance and the statistical moments of asset shocks. Our analysis shows that higher homogeneity in banks' systemic significances requires banks' portfolio holdings to be further away from a full diversification strategy to reduce inefficiencies.

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MS13

When to Stop Supporting Your Bankrupt Subsidiary

Most global banks consist of dozens if not hundreds of subsidiaries. For corporations becoming a holding with subsidiaries has several advantages: It allows them to limit the spillover risk if one business line is in trouble or to defer taxable business income. For example a bank holding may naturally divide into subsidiaries based on location (i.e. Europe, US) and/or business lines (i.e. equity trading, fixed income trading). We consider a network of holding banks. We show that comprising a firms business activity in a holding can have both, positive or negative effects on systemic stability. We analyse to what extent voluntary support benefits society and/or the holding itself. We observe that an increased commitment of the holding to its subsidiaries can have both, positive and negative effects on systemic risk depending on the type of the holding.

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MS13

The Hyperbolic Geometry of Financial Networks

The popularity-vs-similarity model based on hyperbolic geometry has been successfully used to explain the structure of informational, social and biological networks. Just as the geometric structure of a social network determines the diffusion of news, rumors or infective diseases, the geometric structure of a financial network influences the diffusion of financial distress between financial institutions. Indeed, the lack of understanding for risks originating from the systemic interaction of financial institutions has been identified as a major contributing factor to the global financial crisis of 2008. While many recent studies have analysed the mechanisms of financial contagion in theoretical or simulation-based settings, it has remained an open question whether the paradigm of hyperbolic structure applies to financial networks and what such a structure implies for financial contagion processes. In this talk we introduce a new method for embedding distance-based data into hyperbolic space. We show that financial networks inferred from bank balance sheet data can efficiently be embedded into lowdimensional hyperbolic space with considerably smaller distortion than into Euclidean space. We provide a structural decomposition of the embedding coordinates into popularity and similarity dimension and demonstrate that these dimensions align with systemic importance and membership in regional banking clusters respectively.

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MS13

Systemic Risk in Repurchase Agreement Markets

The financial system is increasingly interconnected. Cyclical interdependencies among corporations may cause that the default of one firm seriously affects other firms and even the whole financial network, which is a systemic risk. To describe the connections between banks, many researchers use the uncollateralized liabilities between two firms to construct financial network models of the systemic risk. In practice, there are many collateralized liabilities between banks from the Repurchase Agreement (Repo) Market. Thus it is very important to include the Repo liabilities into the network models. In our research, we apply a Repo liability matrix and an uncollateralized liability matrix to describe the connections between banks. Based on this description, we construct a solvency mechanism to quantify the change of banks assets and the effects to their counterparties. In a numerical study, we compare the effects of the Repo markets on the whole banking system for various financial shocks.

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MS14

Uncertainty Quantification for Hydrodynamics Instabilities in Inertial Confinement Fusion

Hydrodynamic instabilities arise between fluids when an interface is accelerated and are observed in a wide variety of applications such as astrophysical thermonuclear flashes and inertial confinement fusion (ICF). An ICF capsule is filled with multiple layers of fuel, typically composed of deuterium-tritium (D-T), surrounded by a layer of ablator material. The capsule is then compressed to generate the conditions necessary for fusion reactions to occur in the extent of the fuel. The goal is to generate a net excess of energy from this process, known as ignition, making fusion a viable alternative energy source. In the design of ICF capsules, understanding the cause of the failures play an important role in achieving ignition. In this talk, we address the issues to characterize and quantify the effects of uncertainties in model parameters.

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MS14

Cluster Prediction for Opinion Dynamics from Partial Observations

We present a Bayesian approach to predict the clustering of opinions for a system of interacting agents from partial observations. The Bayesian formulation overcomes the unobservability of the system and quantifies the uncertainty in the prediction. We characterize the clustering by the posterior of the clusters' sizes and centers, and we represent the posterior by samples. To overcome the challenge in sampling the high-dimensional posterior, we introduce an auxiliary implicit sampling (AIS) algorithm using two-step observations. Numerical results show that the AIS algorithm leads to accurate predictions of the sizes and centers for the leading clusters, in both cases of noiseless and noisy observations. In particular, the centers are predicted with high success rates, but the sizes exhibit a considerable uncertainty that is sensitive to observation noise and the observation ratio.

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MS14

Uncertainty Quantification in Diffeomorphic Image Registration

We discuss uncertainty quantification in the context of diffeomorphic image registration problems. Our formulation is a non-linear optimal control problem with initial value control; the control variable is the initial momentum (or the initial velocity) at t=0. The partial differential equation (PDE) constraints are the transport equations for the image intensities and the so-called Euler Poincare equations for diffeomorphisms (EPDiff) for the velocity. We exploit problem structure through derivative information of a local Gaussian approximation of the posterior probability density function (PDF). This allows us to efficiently manipulate the associated high-dimensional PDF that arises from the discretization of the corresponding Bayesian inverse problem. We study different numerical schemes to efficiently approximate the associated derivative information in terms of accuracy and computational requirements and make the proposed numerical strategy tractable. We report results for synthetic and real data.

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MS14

Ultrasound Modulated Bioluminescence Tomography with Single Measurement: Inversion and Uncertainty Quantification

Ultrasound modulated bioluminescence tomography (UMBLT) is a hybrid imaging modality where optical measurement is made in the presence of ultrasound modulation in order to identify the distribution of optical sources. While previous reconstructive approaches exist, they require large numbers of optical measurements. In this talk, we will propose an alternative solution to this problem which is able to recover isotropic sources with a single optical measurement. We will derive inversion formulae, show their convergence, and prove uncertainty quantification results. Numerical implementation is included to reconstruct both continuous and discontinuous sources in the presence of noise.

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MS15

Characterizations of the Generalized Inverse Gaussian, Asymmetric Laplace, and Shifted Exponential Laws via Independence Properties

We prove three new characterizations of the generalized inverse Gaussian (GIG), asymmetric Laplace (AL), and shifted exponential (sExp) distributions in terms of non-trivial independence preserving transformations, which were conjectured by Croydon and Sasada. We do this under the assumptions of absolute continuity and natural normality conditions on the densities. Croydon and Sasada use these independence preserving transformations to analyze statistical mechanical models which display KPZ behavior. Our characterizations show the integrability of these models only holds for these three specific distributions in the absolutely continuous setting. Faculty Advisors: Christian Noack, Department of Mathematics, Cornell University, noack@cornell.edu

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MS15

Enhancing Dynamic Mode Decomposition using Autoencoder Networks

Prediction, estimation, and control of dynamical systems remain challenging due to nonlinearity. The Koopman operator is an infinite-dimensional linear operator that evolves the observables of a dynamical system which we approximate by the dynamic mode decomposition (DMD) algorithm. Using DMD to predict the evolution of a nonlinear dynamical system over extended time horizons requires choosing the right observable function defined on the state space. A number of DMD modifications have been developed to choose the right observable function, such as Extended DMD. Here, we propose a simple machine learning based approach to find these coordinate transformations. This is done via a deep autoencoder network. The simple DMD autoencoder is tested and verified on nonlinear dynamical system time series datasets, including the pendulum and fluid flow past a cylinder. Faculty Advisors: Christopher Curtis, San Diego State University, ccurtis@sdsu.edu

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MS15

Distributed-Memory Parallel Algorithm for Solving Integral Equations

In this presentation, we introduce a distributed-memory parallel method for solving systems of linear equations Kx = b, which arises from the discretization of an integral equation. It is well-known that applying a N by N kernel matrix K to a vector can be evaluated with O(N) operations using the fast multipole method (FMM). In addition, recent development has shown that factorizing matrix K can also be done in O(N) operations under appropriate rank assumptions. However, these algorithms still require a significant amount of computation and storage. We introduce a scalable parallel algorithm to solve large-scale problems on distributed-memory machines. Our parallel algorithm exploits the same hierarchical decomposition of the problem domain as in the (parallel) FMM. The decomposition is naturally associated with a quad-/oct-tree data structure, where the work required for every tree node is almost constant and the calculation is local—as in the FMM. A key feature of our parallel algorithm is that every processor requires only local communication. Faculty Advisors: George Biros, UT Austin, biros@oden.utexas.edu

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MS15

Multigrid for Fourier Finite Element Methods on Axisymmetric Domains

H(curl)-problems defined on a three-dimensional axisymmetric domain can be reduced to a sequence of weighted two-dimensional (2D) problems by using a partial Fourier series decomposition. The term Fourier finite element methods (FEMs) is used when an adequate FEM is used to approximate the solution to each of these weighted 2D problems. In this talk, we will numerically show that the multigrid V-cycle algorithm with modern smoothers will converge uniformly with respect to meshsize when applied to these weighted H(curl)-problems. This work was done during the Summer@ICERM2020 program at Brown University. Faculty Advisors: Minah Oh, James Madison University, ohmx@jmu.edu; Yanlai Chen, University of Massachusetts, Dartmouth, yanlai.chen@umassd.edu This talk will be presented by both Yonah Moise and Trevor Crupi.

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MS15

How Fast Can You Make Gradients Small? A Potential Function-Based Study of Classical and Recent Algorithms

First-order methods designed to make the gradients small are at the heart of many applications in optimization and machine learning. For example, they play a central role in finding parameter-free algorithms and they can provide stronger guarantees both in terms of feasibility and optimality gap for certain linearly constrained problems. However, many basic questions about these algorithms still remain unsolved, including finding a general framework to analyze the behavior and iteration complexity of these algorithms. Our paper (arXiv:2101.12101) proposed a potential function-based framework to address this important question. In this presentation, I will discuss how this framework can be intuitively applied to the study of the convergence rates of a number of algorithms in different settings, including: (i) in convex optimization, classical gradient descent and the recent optimal OGM-G algorithm, and (ii) in convex-concave min-max optimization, gradient descent-ascent and Halpern iteration. In general, the framework can be interpreted as a tradeoff between reducing either gradient norm or the optimality gap. I will further complement these results with a discussion of the optimality of gradient descent-ascent and Halpern iteration among a large class of algorithms, based on a new lower bound for minimizing the norm of cocoerceive operators, obtained as part of our work. Faculty Advisors: Jelena Diakonikolas, UW Madison, jelena@cs.wisc.edu

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MS15

Implementation of Mixed Precision Arithmetic in Regularization Methods

In numerical computations, using low precision floating point arithmetic enables computer programs for scientific applications to have faster loops, less communication, and lower energy consumption. As low precision arithmetic leads to limited accuracy for certain data, a mixed precision approach uses low precision arithmetic to accelerate speed on certain calculations, mixed with a limited amount of high precision calculations, while maintaining sufficient accuracy of the final result. Recent work by Higham and colleagues studies the use of mixed precision arithmetic for algorithms to solve certain basic, well-conditioned linear systems. In my presentation, we extend these ideas to the more complicated class of inverse problems, where regularization techniques, such as truncated singular value decomposition (TSVD) and Tikhonov regularization, are needed to compute an approximate solution of a severely ill-conditioned problem. We implement different methods, such as generalized cross validation (GCV), to help estimate good regularization parameters under mixed precision arithmetic and use Iterated Tikhonov to further improve the accuracy. Faculty Advisors: James Nagy, Emory University, jnagy@emory.edu

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MS16

Inverse Random Potential Scattering for Elastic Waves

This talk is concerned with the inverse elastic scattering problem for a random potential in three dimensions. Interpreted as a distribution, the potential is assumed to be a microlocally isotropic Gaussian random field whose covariance operator is a classical pseudo-differential operator. Given the potential, the direct scattering problem is shown to be well-posed in the distribution sense by studying the equivalent Lippmann-Schwinger integral equation. For the inverse scattering problem, we demonstrate that the microlocal strength of the random potential can be uniquely determined with probability one by a single realization of the high frequency limit of the averaged compressional or shear backscattered far-field pattern of the scattered wave. The analysis employs the integral operator theory, the Born approximation in the high frequency regime, the microlocal analysis for the Fourier integral operators, and the ergodicity of the wave field.

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MS16

Fast Signal Recovery from Quadratic Measurements

We present a novel approach for recovering a sparse signal from quadratic measurements corresponding to a rank-one tensorization of the data vector. Such quadratic measurements, referred to as interferometric or cross-correlated data, naturally arise in many fields such as remote sensing, spectroscopy, holography and seismology. Compared to the sparse signal recovery problem that uses linear measurements, the unknown in this case is a matrix, $X = \rho\rho^*$, formed by the cross correlations of $\rho \in C^K$. This creates a bottleneck for the inversion since the number of unknowns grows quadratically in K. The main idea of the proposed approach is to reduce the dimensionality of the problem by recovering only the diagonal elements of the unknown matrix, $|\rho_i|^2$, $i = 1, \ldots, K$. The contribution of the off-diagonal terms $\rho_i\rho_j^*$ for $i \neq j$ to the data is treated as noise and is absorbed using the Noise Collector approach introduced in [Moscoso et al, The noise collector for sparse recovery in high dimensions, PNAS 117 (2020)]. With this strategy, we recover the unknown by solving a convex linear problem whose cost is similar to the one that uses linear measurements. The proposed approach provides exact support recovery when the data is not too noisy, and there are no false positives for any level of noise.

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MS16

Differential Faraday Rotation and Polarimetric SAR

The propagation of linearly polarized electromagnetic waves through the Earth's ionosphere is accompanied by Faraday rotation (FR), which is due to gyrotropy of the ionospheric plasma in the magnetic field of the Earth. FR may cause distortions of the images taken by spaceborne polarimetric synthetic aperture radars (SAR). We show that the mechanism of those distortions is related to the variation of the FR angle within the bandwidth of the interrogating signals sent by the radar. This effect has not been analyzed previously in the context of SAR imaging. We also propose a special matched filter that we call the polarimetric matched filter (PMF). The PMF helps correct the FR-induced distortions and provides a provably superior SAR performance compared to the case of the traditional polarimetric SAR signal processing.

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MS17

Pulmonary Imaging with Combined Ultrasound and Electrical Impedance Tomography Data

Electrical impedance tomography (EIT) and low-frequency ultrasound computed tomography (USCT) are two imaging modalities which both have the potential to allow fast and portable pulmonary monitoring with no ionizing radiation. Each method has its own strengths and drawbacks: EIT has excellent interior signal propagation but low spatial resolution, while USCT allows for sharper images but suffers from poor signal penetration. We therefore present a hybrid EIT-USCT methodology wherein data for the two modalities are collected in tandem, and we combine the strengths of each technique via the complementary use of priors. The method is validated using reconstructions of simulated pulmonary data.

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MS17

Progress on Simultaneous Multiple Source EIT

Electrical Impedance Tomography (EIT) is a non-invasive, real-time functional imaging modality and appropriate for medical application especially on pediatric and neonatal patients. Since 2000, multiple studies have demonstrated EITs potential for bedside monitoring of ventilation in infants. Although the spatial resolution of EIT is not comparable to that of a CT scan, its temporal resolution is excellent. All commercial EIT systems, produced by Drager, SwissTom, Timpel and others, use a single or bipolar current source and spatial multiplexing. However, single and bipolar EIT systems have drawbacks that include: 1) significantly inferior ability to detect small inhomogeneities (regardless of the choice of algorithm); 2) limited ability to detect perfusion signals which are 10 20 times smaller than the ventilation signal. Simultaneous Multi Source (SMS) EIT is significantly better than single/bipolar EIT because it has higher sensitivity and can detect small inhomogeneities in ventilation and perfusion. GE Research developed a high-precision SMS-EIT prototype system, consisting of 32 independently driven currents and voltage meters with 16-bit accuracy at 20 50 frames per second with different settings. Because of this high sensitivity, we were able to provide noninvasive, real-time lung function monitoring with breath-to-breath regional ventilation and beat-to-beat perfusion information without using any contrast agents, ionizing radiation or signal averaging processes.

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MS17

A Bayesian Filtering Approach to Stable Layer Stripping Algorithm for EIT

Several direct computational methods (e.g. Layer Stripping, D-bar Method) are available for reconstructing electric conductivity distributions from current-voltage (Neumann to Dirichlet (NtD)) continuous boundary data. In particular, Layer Stripping algorithm is a direct numerical method capitalizes on back propagating the nonlinear differential equation of Riccati type satisfied by the NtD map while approximating the conductivity. However, the Riccati equation while back propagating is prone to encounter numerical instabilities in a finite time. In this talk, we propose an efficient computational method to approximate the conductivity by excluding the back propagation of the unstable Riccati equation based on well-known Kalman filtering techniques. Moreover, we show the adaptability of the proposed method and the reconstruction results from the KIT4 measurement data.

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MS17

A Three Dimensional Calderon-Based Method for EIT on the Cylindrical Geometry

Objective: Electrical impedance tomography (EIT) is an imaging modality in which voltage data arising from currents applied on the boundary are used to reconstruct the conductivity distribution in the interior. This paper provides a novel direct (noniterative) 3-D reconstruction algorithm for EIT in the cylindrical geometry. Methods: The algorithm is based on Calderón's method [Calderón, 1980], and is implemented for data collected on two or four rows of electrodes on the boundary of a cylinder. Results: The effectiveness of the method to localize inhomogeneities in the plane of the electrodes and in the z-direction is demonstrated on simulated and experimental data. Conclusions and Significance: The results from simulated and experimental data show that the method is effective for distinguishing in-plane and nearby out-of-plane inhomogeneities with good spatial resolution in the vertical z direction with computational efficiency.

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MS18

New Integrable Peakon Equations

Peakons are peaked travelling waves that were first found as solutions to the Camassa-Holm equation arising in the theory of shallow water waves. The Camassa-Holm equation is an integrable system which possesses multi-peakon solutions. These discoveries started an extensive study of peakon equations, both integrable and non-integrable. This talk will survey some recent work on a search for new integrable equations: (i) multi-peakon solutions exist for a wide class of nonlinear dispersive wave equation and does not require integrability; (ii) new integrable peakon equations exhibiting parity-time non-invariance have been obtained (iii) many integrable peakon equations arise as reductions of certain universal multi-component peakon integrable systems.

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MS18

Curved Soliton and Its Interaction for KP Equation

The curved soliton solutions for KP equation are studied by using the direct method in soliton theory. Interactions between curved solitons, line solitons and breather solutions are also investigated analytically. Following the construction of special function solutions for integrable nonlinear evolution equations, the tau functions of the solutions are explicitly given in the determinant form.

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MS18

Norming Constants of Embedded Bound States

and Bounded Positon Solutions of the Korteweg-De Vries Equation

In the context of the full line Schrodinger equation, we put forward a new type of the binary Darboux transformation which inserts or removes any number of positive eigenvalues embedded into the absolutely continuous spectrum without altering the rest of scattering data. We then show that embedded eigenvalues produce an additional explicit term in the KdV solution. This term looks similar to multi-soliton solution and describes waves traveling in the direction opposite to solitons. It also resembles the known formula for (singular) multi-positon solutions but remains bounded, which answers in the affirmative Matveev's question about existence of bounded positons.

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MS18

Universal Patterns of Rogue Waves in Integrable Systems

We show that universal rogue wave patterns exist in integrable systems. These rogue patterns comprise fundamental rogue waves arranged in shapes such as triangle, pentagon, heptagon and nonagon, with a possible lower-order rogue wave at the center. These patterns appear when one of the internal parameters of bilinear rogue waves gets large. Analytically, these universal patterns are given by the root structures of the Yablonskii-Vorobev polynomial hierarchy through a linear transformation. Thus, the induced rogue patterns in the space-time plane are simply the root structures of Yablonskii-Vorobev polynomials under actions such as dilation, rotation, stretching and translation. As examples, these universal rogue patterns are explicitly determined and graphically illustrated for the nonlinear Schrodinger equation, the derivative nonlinear Schrodinger equation, the Boussinesq equation, and the Manakov system.

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MS19

Medical Time Series Collected in Free Living Environments: Data Quality and Patient Heterogeneity

Bio-sensors are increasingly popular tools to collect data in the behavioral sciences. Instead of being bound to lab settings, off-the-shelf wearable devices allow the collection of observational data in participants' daily living environment. This introduces new opportunities and challenges to the collection, curation, and analysis of such sensor data. In this talk, we will exemplify these opportunities and challenges by an observational study at a Dutch nursing home. Residents activity data and location information was collected with wearables, and data from fixed sensors (i.e., domotica) was obtained to observe residents daily life. The sensor data enriches the observations on residents' behavior by field experts and allows for intensive data collection over a longer time period. From a data science and analysis point of view, questions arise concerning the quality of this data. We will discuss how the heterogeneity of the residents disease state affects data quality. Data quality will depend on residents fluctuating mental state and willingness to participate in the study. Furthermore, using off-the shelf wearables on a niche population with very low activity levels poses challenges to the interpretation of the data generated by black-box models on the wearable itself (e.g., heart rate or activity classes). Lastly, we will show how these data quality issues can propagate through analysis pipelines and what that means for small-scale observational studies.

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MS19

Bayesian Approaches to Data Interpretation in Applied Physical Sciences

Fluorescence experiments based on Förster resonance energy transfer **(FRET)** present a powerful way to probe switching kinetics between the conformational states of a molecule. The acquired data from these experiments generated by a single molecule are traditionally interpreted with hidden Markov models (HMMs). The underlying modeling assumptions for HMM framework is that the switching kinetics of the molecule has to be slower compared to the data acquisition rate. The problem is, single molecule kinetics are unknown in principle. Therefore, it is unclear, a priori, whether HMM framework applies to the probed single molecule kinetics. In this talk, I will present an overview of what we propose for the generalization of HMMs for single molecules as they switch between their conformational states. I will demonstrate a variant of HMM generalization performance on experimental data from FRET labeled Holliday junctions. I will also highlight the novel Bayesian non-parametric approaches on how to tackle with the model selection problem when the conformational states of the molecule are unknown.

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MS19

Analyzing Clinical and Biological Data for Disease Detection

We analyze clinical and biological data using anomaly detection to identify disease related events. The datasets analyzed include data from an ongoing collection from participating clinics as well as existing datasets. We look at challenges related to applying these methods on real datasets.

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MS19

Machine Learning for Triage Recommendations

Viral and chronic respiratory illnesses are characterized by rapid health deterioration episodes that manifest as either emergency care events (in the case of chronic lung disease) or rapid infection spread (in the case of Covid-19 and Influenza). In this study, we present an approach to identifying clinically significant flare-ups of respiratory illness using globally available clinical characteristic data and physician provided triage labels. The methodology leverages Bayesian Inference and Monte Carlo methods to generate hypothetical patient scenarios for training triage algorithms. Machine-learning prediction models are evaluated in out-of-sample validation tests of accuracy, sensitivity, specificity, ppv, and npv when detecting health deterioration and recommending the most appropriate responsive care. Algorithm recommendation and exacerbation identification time series data from real patient trials is then used to risk stratify chronic lung patients for future health downturns using signature methods coupled with classical machine-learning.

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MS20

Optimal Transport in Kyle's Model of Informed Trading

We show connections between optimal transport theory and the dynamic version of the Kyle model, including new characterizations of informed trading profits via the conjugate of the Brenier potential and Monge-Kantorovich duality. Using results from optimal transport theory, we extend the Kyle model to scenarios with multiple assets, general asset distributions, and risk-averse market makers. In an application of the general model, we show that, when there is informed trading in options and an underlying asset and market makers are risk averse, option-implied volatilities predict the return of the underlying asset. Based on joint work with Kerry Back, Francois Cocquemas and Abraham Lioui.

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MS20

Unequal Dimensional Optimal Transport and Applications in Economic Theory

This talk focuses on optimal transport problems in which the dimension of the source measure is larger than that of the target. Until recently, these problems have received relatively little attention in the mathematics literature but are very natural in economics, where, for example, optimal transport is used to model matching markets in which the dimensions of heterogeneity on the two sides of the market differ. We describe a general approach to solve problems where the source is multi-dimensional and the target unidimensional. If time permits, we will briefly discuss the extension to the case where the target is multi-dimensional (but still lower dimensional than the source), as well as problems in which one of the marginals is free while the other is fixed, motivated in part by the study of Cournot-Nash equilibria. This talk represents various joint works with Pierre-Andre Chiappori, Robert McCann and Luca Nenna.

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MS20

Modeling the Capital Distribution Curve: Optimal Transport and Dimension Reduction

The capital distribution curve gives the ranked portfolio weights of the market portfolio. It exhibits long-term stability which is of great interest in stochastic portfolio theory. In the first part of the talk we study its stability relative to its name-based counterpart using a Wasserstein metric. Next we consider dimension reduction of the capital distribution curve using the Aitchison geometry of the simplex and a methodology called convex principal component analysis (cPCA). We show that the first principal component can be interpreted in terms of market diversity, hence giving a statistical justification of the concept. This is an on-going project with Steven Campbell.

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MS21

Iteration for Contour-Based Nonlinear Eigensolvers

Contour integration techniques have become a popular choice for solving the linear and non-linear eigenvalue problems. They principally include the Sakurai-Sugiura methods, the Beyn's algorithm, the FEAST/NLFEAST algorithms and other rational filtering techniques. While these methods can result in effective 'black-box' approaches for solving linear eigenvalue problems, they still present several shortcomings for addressing nonlinear eigenvalue problems which are both mathematically and practically far more challenging. We introduce a new hybrid algorithm that advantageously combines the iterative nature of NLFEAST with the effectiveness of Beyn's approach to deal with general non-linearity. In doing so, this NLFEAST-Beyn hybrid algorithm can overcome current limitations of both algorithms taken separately. After presenting its derivation from both a Beyn's and NLFEAST's perspective, several numerical examples are discussed to demonstrate the efficiency of the new technique.

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MS21

Spectral Calculations for Magic Angles in a Simple Model of Twisted Bilayer Graphene

Tarnopolsky, Kruchkov, and Vishwanath have proposed a simplified model of twisted bilayer graphene based on a Hamiltonian that is periodic with respect to a special two-dimensional lattice. The spectral behavior of this model can be understood in terms of a non-self-adjoint operator $D(\alpha)$, which depends on the angle $1/\alpha$ that describes the orientation of the two graphene sheets. For most values of α the spectrum of $D(\alpha)$ is a constant discrete set in the complex plane; however, for special "magic" values of α the spectrum is the entire complex plane. We illustrate this behavior by studying the pseudospectra of $D(\alpha)$ and conducting a variety of other spectral calculations that investigate the separation of magic α values and crucial properties of the potential.

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MS21

Randomized Feast Algorithm

Next generation algorithms for solving fundamental problems of linear algebra, i.e., linear systems, least-squares or eigenvalue problems, will need to significantly reduce the amount of data pulled into the memory, e.g. by examining only a subset of the input matrix, minimize communication, and allow decentralized processing and communication algorithms. computations. Of particular interest to us are randomized algorithms for eigenvalue computations. In this talk, we will present a randomized eigenvalue solver based on contour integration, i.e., the randomized FEAST algorithm. We will concentrate on the probabilistic error analysis of the algorithm and practical implications of proposed error bounds. This is a joint work with Nikita Kapur (KU) and Arvind Saibaba (NCSU).

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MS21

Computing the Spectra of Differential Operators

Spectral methods for solving differential eigenproblems usually follow the "discretize-then-solve" paradigm. Discretize first, and then solve the matrix eigenproblem. The discretize-then-solve paradigm can be tricky for differential eigenproblems as the spectrum of matrix discretizations may not converge to the spectrum of the differential operator. Moreover, it is impossible to fully capture the continuous part of the spectrum with a finite-sized matrix eigenproblem. In this talk, we will discuss an alternative "solve-then-discretize" paradigm for differential eigenproblems. To compute the discrete spectrum, we will discuss a continuous analogue of FEAST by approximating the action of the resolvent operator. For the continuous spectra, we will use a Cauchy-like integral to calculate a smoothed version of the so-called spectral measure.

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MS22

Function Space Random Feature Methods for Learning Parametric PDE Solution Operators

Recently, a line of research has emerged regarding the supervised learning of mappings between infinite-dimensional spaces of functions. In this work, we propose a data-driven randomized algorithm that falls within this overarching framework. Specifically, we extend the classical random feature model as an approximation architecture operating between finite-dimensional vector spaces to one operating between function spaces. The primary input-output mappings of this type that motivate our work are solution operators of partial differential equations (PDE) parametrized by random input functions. The proposed method, which can be viewed as a random parametric approximation of nonparametric operator-valued kernel ridge regression, is conceptually defined in infinite dimensions and as a result, in practice can be deployed across different finite-dimensional discretizations of the input and output function spaces without the need for re-training. We enhance our random feature method with prior knowledge from the underlying PDEs and numerically demonstrate its approximation accuracy and robustness to choice of discretization dimension for parametric PDE forward solution operators, and conclude with its application as a surrogate model for Bayesian inverse problems.

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MS22

Train Like a (Var)Pro: Efficient Training of Neural Networks using Variable Projection with Applications in Surrogate Modeling

The success and flexibility of deep neural networks (DNNs) have motivated their use in scientific applications, such as partial differential equation (PDE) surrogate modeling. For these scientific applications, it is essential to train networks that produce highly-reliable models. In this talk, we will discuss our Gauss-Newton-based algorithm for training DNNs to high accuracy, GNvpro. Our method extends the use of variable projection (VarPro), originally designed for separable least squares, to non-quadratic loss functions, making it effective for, e.g., classification. Additionally, GNvpro is nearly-independent of the DNN architecture and hence can train many state-of-the-art DNNs. Through two PDE surrogate modeling tasks, we will demonstrate that GNvpro not only solves the optimization problem more efficiently but also yields DNNs that generalize better than commonly-used optimization schemes.

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MS22

Derivative Informed Projected Neural Networks for High Dimensional Parametric PDE Maps

Outer-loop problems arising in scientific applications (such as optimization, uncertainty quantification and inverse problems) require repeated evaluation of computationally intensive numerical models, such as those arising from discretization and solution of ordinary and partial differential equations. The cost of these evaluations makes solution using the model prohibitive, and efficient accurate surrogates are a key to solving these problems in practice. In this talk we will investigate how low dimensional derivative information can be used to construct parsimonious encoder-decoder neural networks that have weight dimensions that can be made independent of the discretization dimension. These compact representations require relatively few data to train and outperform conventional data-driven approaches which require large training data sets. This methodology can be easily adapted to derivative training, where the surrogate can be used to approximate derivative information used in inference or optimization applications.

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MS22

Solving Inverse Problems with Deep Learning

This talk is about some recent progress on solving inverse problems using deep learning. Compared to traditional machine learning problems, inverse problems are often limited by the size of the training data set. We show how to overcome this issue by incorporating mathematical analysis and physics into the design of neural network architectures. We first describe neural network representations of pseudodifferential operators and Fourier integral operators. We then continue to discuss applications including electric impedance tomography, optical tomography, inverse acoustic/EM scattering, seismic imaging, and travel-time tomography.

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MS23

The Price of the Edge: An Analytical Model

Edge computing is key to enabling applications running on resource constrained devices such as IoT devices to offload latency-critical computations to a pool of nearby resources. However, there has been limited work on modeling edge clouds to better understand how they compare to centralized large-scale back end clouds in terms of performance and cost. In this work, we will present some of our analytical models for edge computing as distributed queues, comparing them to centralized queue. We provide closed-form queuing models that enable designers to study the cost-performance trade-offs with respect to the provisioning of both systems, and how workload variations, service time distributions of the servers, and workload mobility affects these trade-offs.

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MS23

Stochastic Multicast Routing Protocol for Flying Ad-Hoc Networks

Wireless ad-hoc network is a decentralized type of temporary machine-to-machine connection that is spontaneous or impromptu so that it does not rely on any fixed infrastructure and centralized administration. As unmanned aerial vehicles (UAVs), also called drones, have recently become more accessible and widely utilized in military and civilian domains such as surveillance, search and detection missions, traffic monitoring, remote filming, product delivery, to name a few. The communication between these UAVs become possible and materialized through Flying Ad-hoc Networks (FANETs). However, due to the high mobility of UAVs that may cause different types of transmission interference, it is vital to design robust routing protocols for FANETs. In this talk, the multicast routing method based on a modified stochastic branching process is presented. The reproductive number in stochastic branching model is used to regulate the local transmission rate is adapted and modified for flying ad-hoc network communication. Besides, the improved adaptive transmission models are introduced. We compare the proposed method with flooding method for their performance.

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MS23

Efficient Edge Computing for Mobile Internet of Things in Wireless Networks

In recent years, a significant growth of network connected devices such as smart phones, tablets, laptops, automobiles and drones has been witnessed from the development of Internet of Things (IoT). This growth results in the use of tens of billions of devices, which require a massive quantity of computational processing and storage resources for sensory data of the environment in autonomous driving, graphics rendering for online gaming, video streaming and more. Here, we study the efficient edge computing (EEC) problem for a joint computing to process a task both locally and remotely with the objective of minimizing the finishing time. When computing remotely, the time will include the communication and computing time. We describe the time model, formulate EEC, prove NP-completeness of EEC, and show the lower bound of the problem. We then provide an integer linear programming (ILP) based algorithm to achieve the optimal solution and give results for small-scale cases. A fully polynomial-time approximation scheme (FPTAS), named Approximation Partition (AP), is provided through converting ILP to the subset sum problem. FPTAS refers to a type of approximation algorithm which runs in polynomial and achieves the approximation ratio within 1+?? for a given error ??. Numerical results show that both the total data length and the movement have great impact on the finishing time for edge computing. Numerical results also demonstrate that our AP algorithm obtain the finishing time, which is close to the optimal solution.

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MS24

Mean Field Portfolio Games in Ito Diffusion Markets under Competition

In this talk, I will discuss two families of N-agent and mean-field games for optimal investment in Ito-diffusion markets under relative performance concerns. The first family considers incomplete markets with exponential preferences while the second looks at complete markets but with stochastic exponential risk tolerance coefficients. For both cases, the optimal policies, optimal wealth processes and value function are given in closed forms. Explicit solutions are also constructed for representative Markovian cases.

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MS24

Convergence of Large Population Games to Mean Field Games with Interaction through the Controls

This work considers stochastic differential games with a large number of players, whose costs and dynamics interact through the empirical distribution of both their states and their controls. We develop a new framework to prove convergence of finite-player games to the asymptotic mean field game. Our approach is based on the concept of propagation of chaos for forward and backward weakly interacting particles. These propagation of chaos arguments together with new functional inequalities further allow to derive moment and concentration bounds for the convergence of both Nash equilibria and social optima in non-cooperative and cooperative games, respectively. The talk is based on join works with M. Lauriere and D Bartl.

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MS24

Optimal Dynamic Contracts with Environmental, Social and Governance Criteria

We examine dynamic contracts when output has negative environmental effects and the manager (agent) can invest to build up ESG capital and mitigate the externality. The incentive component of the optimal contract rewards based on cash flow and ESG capital when the principal is risk neutral; and it additionally loads on the production externality when the principal has CARA. Optimal ESG contracts are less sensitive to traditional pay-for-performance measures, and ESG investment is determined by the ratio of capital to cash flow exposure in the contract. We identify conditions under which ESG investment is optimal and improves welfare. We also examine constrained contracts controlling the agency friction associated with ESG investment.

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MS24

Mutual Funds Competition for Investment Flows based on Relative Performance

N mutual funds compete for fund flows based on relative performance over their average returns, by choosing between an idiosyncratic and a common risky investment opportunities. The unique constant equilibrium is derived in closed form, which implies that funds generally decrease the investments in their idiosyncratic risky assets under competition, in order to lower the risk of the relative performance. It pushes all funds to herd and hurts their after-fee performance. However, the sufficiently disadvantaged funds with poor idiosyncratic investment opportunities or highly risk averse managers may take excessive risk for a better chance of attracting new investments, and their performance may improve comparing to the case without competition and benefits the investors.

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MS25

Nvshmem: A Partitioned Global Address Space Library for Nvidia GPU Clusters

NVSHMEM is an implementation of the OpenSHMEM parallel programming model for clusters with NVIDIA GPUs. NVSHMEM allows the programmer to aggregate the memory of multiple GPUs into a Partitioned Global Address Space (PGAS) that supports transparent remote access through one-sided get, put, and atomic update operations over InfiniBand, PCI Express, and NVLink interconnects. With NVSHMEM, it is possible to initiate communication from the CPU, on CUDA streams and graphs, and from within a CUDA kernel. Through application case studies, we show that integrating the communication model with the GPU's execution model can improve programmability and reduce overheads. GPU initiated communication takes advantage of the GPU execution model to naturally hide communiation latencies using multithreading. It can also eliminate kernel boundaries induced by communication models that initiate communication from the CPU. NVSHMEM's CUDA stream and graph initiated communication integrates with the GPU work scheduling model and can help to hide offloading overheads. By reducing synchronization with the CPU and supporting fine-grained communication that naturally overlaps with computation, NVSHMEM can provide better strong scaling efficiency than the predominant CPU initiated communication models used by most HPC applications today.

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MS25

Roc_shmem: a GPU-Centric Openshmem

Current state-of-the-art in GPU networking utilizes a host-centric, kernel-boundary communication model that reduces performance and increases code complexity. To address these concerns, we introduce ROC_SHMEM, a GPU centric PGAS programming model and runtime that enables Intra-kernel communication. ROC_SHMEM enables fine-grain computation-communication overlap by allowing the GPU threads to directly perform network operations without the need of ending the GPU kernel. In this talk we will present the ROC_SHMEM programming model, its architecture, and its different runtime conduits. We illustrate that for structured applications like a Jacobi 2D stencil, ROC_SHMEM can improve application performance by up to 40% compared to traditional kernel-boundary networking. Furthermore, we demonstrate that on irregular applications like Sparse Triangular Solve (SpTS), ROC_SHMEM provides up to 44% improvement compared to existing intra-kernel networking schemes.

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MS25

Towards Portable PGAs on GPUs

GPUs have become an essential component for next-generation high-performance computer clusters. To efficiently move data between GPUs on such clusters, we investigate the Partitioned Global Address Space (PGAS) approach for GPUs and propose a portable implementation. We use the SYCL programming framework to support multiple types of GPU, and MPI-3 one-sided operations are used for distributed memory communication on different network architectures. We implement a 2D stencil kernel using our newly implemented GPU PGAS library and compare its performance with a CUDA-aware MPI-based implementation and an NVSHMEM (an OpenSHMEM implementation specialized for NVIDIA GPU and InfiniBand network) implementation. Test results show that our implementation is faster than the CUDA-aware MPI-based implementation, and the inter-node communication latency is critical to the performance and scalability of PGAS on GPUs.

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MS25

OSHMPI: OpenSHMEM over MPI for Portable and Efficient GPU Communication

OpenSHMEM is an increasingly popular standard of the SHMEM programming model. OpenSHMEM defines specialized APIs for fast one-sided and collective communication. The intent is to directly map the application communication requests to low-level network API to ensure high performance. Unlike OpenSHMEM, MPI is designed to provide comprehensive features for various data movement patterns over distributed memory systems so that complex algorithms can be written by using MPI. The OSHMPI project aims to investigate the ways to provide a portable and performance-efficient OpenSHMEM library over MPI runtime system. Nowadays, GPUs have become a promising architecture for supercomputing systems. Most GPU-enhanced applications today extend the original CPU-based code by offloading heavy floating-point computations to GPU devices and leaving the remaining code as is. When scaling the applications across computing nodes, the data movement between GPUs and between GPU and host memory has to be taken into account. OSHMPI supports efficient GPU-aware OpenSHMEM communication for such applications by leveraging highly optimized GPU communication provided through the low-level MPI implementations. In this talk, we will introduce the GPU-aware OSHMPI library and discuss several optimizations that we made in the software path of OSHMPI as well as the low-level MPI runtime.

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MS26

Tom Coleman's Journey into Computational Finance

Tom Coleman and I both started working in computational finance in 1995. I came from a PDE background, Tom was an optimization guy. Computational finance is all about optimal stochastic control, so Tom and I had different perspectives on financial problems. I will relate how our paths crossed in such areas as policy iteration for optimal control, high performance computing for option pricing, hedging under jump diffusion processes, variable annuities and finally machine learning.

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MS26

Graph Algorithms in Optimization and the Origins of Combinatorial Scientific Computing

Tom Colemans research interests were broad and interdisciplinary. In the early years of his career he made important contributions by applying combinatorial ideas to problems in continuous optimization. His best-known work in this area is his and Mores recognition that graph coloring is a natural abstraction for exploiting sparsity structure when computing Jacobians and Hessians. But his interest in discrete / continuous fusion also played out in different ways in the research conducted by several of his early PhD students. In this talk I will briefly synopsize some of this work, and then discuss the longer-term impact of this line of work and of the research environment that Tom inculcated. Specifically, there is a very direct line from Toms research and mentoring to the creation of the research community now known as Combinatorial Scientific Computing.

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MS26

Model Calibration: Inversing, Data Learning, and Machine Learning

Tom always believed that one of the most meaningful rewards of research is to see it solving real world problems. Tomdevoted significant focus and effort towards achieving this goal by turning theoretical research into software.In addition, pursuing new research directions driven byapplications had always brought him excitement and satisfaction. In this talk, I will review some research in calibrating a local volatility function for a financial derivative model, my first joint work with Tom in the field of computational finance more than 30 years ago. We viewed this inverse problem as an implicit machine learning problem and handled its regularization using knots placement of interpolating splines, as well as spline kernel with 1-norm regularization. I will also discuss some recent progress using deep learning for on-line option model calibration.

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MS26

Sequential Learning for Price Impact in Optimal Portfolio Execution

Optimal trading strategies often rely on assumptions about the models and their associated parameters to be estimated. Particularly, in illiquid markets and for large-volume trades, specifying the price impact model is essential. This talk discusses this challenge for the optimal portfolio execution problem, which aims to liquidate large blocks of assets over a finite time horizon to minimize the execution cost. We first present results on the sensitivity of the optimal strategy to estimation errors in the price impact parameters. Next, a sequential learning procedure involving a finite set of optimally designed test trades is proposed to improve price impact estimations.

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MS26

Tom Colemans Contributions to Combinatorial Scientific Computing

Tom Coleman, together with Jorge More, pioneered the use of graph coloring algorithms for computing sparse Jacobians and Hessians for the solution of nonlinear problems in the early 1980s. This work was begun during his postdoctoral research at Argonne National Laboratory, and continued together with several of his students at Cornell and Waterloo. He developed several graph coloring models, including distance-1, distance-2, star, and acyclic coloring models, for Jacobian and Hessian estimation based on how sparsity and symmetry were exploited, and what granularity of computation was adopted (rows, columns or both). Toms work was the foundation on which others built to design space- and time-efficient algorithms for these problems. This work was the harbinger of the use of other graph algorithms in scientific computing, such as matching for sparse null space basis computations, automatic differentiation, predicting data structures for sparse orthogonal factorizations, etc., and led to the foundation of the combinatorial scientific computing community in the 2000s.

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MS26

Tom Colemans Contributions to Constrained Nonlinear Optimization

Tom Coleman made important contributions to nonlinear programming during an important time in the development of the field, when interior-point methods were arriving on the scene. Along with collaborator Yuying Li, he proposed methods that incorporate the novel idea of reflection, along with such other elements as second-order information, interiority, and trust regions. With Andy Conn, Tom also investigated the properties of exact penalty function formulations. He was instrumental in founding and developing the Matlab Optimization Toolbox which, for an enormous number of users, is the main way that they interact with optimization technology. This talk will summarize these contributions and their impact on optimization and its community of users.

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MS27

Deep Residual Learning via Large Sample Mean-Field Stochastic Optimization

We study a class of stochastic optimization problems of the mean-field type arising in the optimal training of a deep residual neural network. We consider the sampling problem arising from a continuous layer idealization, and establish the existence of optimal relaxed controls when the training set has finite size. The core of our paper is to prove the Gamma-convergence of the sequence of sampled objective functionals, i.e., show that as the size of the training set grows large, the minimizer of the sampled relaxed problem converges to that of the limiting optimization problem. We connect the limit of the large sampled objective functional to the unique solution, in the trajectory sense, of a nonlinear Fokker-Planck-Kolmogorov (FPK) equation in a random environment. We construct an example to show that, under mild assumptions, the optimal network weights can be numerically computed by solving a second-order differential equation with Neumann boundary conditions in the sense of distributions.

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MS27

Machine Learning Computations for Financial Applications of Multiple Optimal Stopping Problems

Options and contracts with multiple exercises of American type are prevalent in the financial and insurance industry. After reviewing the most popular numerical methods used to value standard American puts, we introduce a neural network architecture to compute the solutions of optimal multiple stopping problems, and demonstrate its efficiency on several examples.

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MS27

Reservoir Optimal Stopping

This paper presents a new approach to solve the optimal stopping problem. The key idea of this approach is to use deep neural networks where the hidden layers are generated randomly and only the last one is trained. Hence, this approach is applicable for high dimension problems where the traditional least-squares Monte Carlo approaches become impractical. In addition, as only a linear regression is needed, this approach is very easy to implement and theoretical guarantees are provided. We illustrate this technique in several realistic examples.

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MS27

Portfolio Optimisation within a Wasserstein Ball a Reinforcement Learning Approach

We consider the problem of active portfolio management where a loss-averse and/or gain-seeking investor aims to outperform a benchmark strategy's risk profile while not deviating too much from it. Specifically, an investor considers alternative strategies that have terminal wealth that lie within a Wasserstein ball surrounding the benchmarks. The investor then chooses the alternative strategy that minimises a distortion risk measure. We develop a reinforcement learning paradigm for solving this problem using risk-aware policy gradient methods and explore various risk-reward tradeoffs.

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MS28

Wave Propagation in Inhomogeneous Media: A New Family of Generalized Plane Waves

Trefftz methods rely, in broad terms, on the idea of approximating solutions to Partial Differential Equation (PDEs) using basis functions which are exact solutions of the PDE, making explicit use of information about the ambient medium. But wave propagation problems in inhomogeneous media is modeled by PDEs with variable coefficients, and in general no exact solutions are available. Generalized Plane Waves (GPWs) are functions that have been introduced, in the case of the Helmholtz equation with variable coefficients, to address this problem: they are not exact solutions to the PDE but are instead constructed locally as high order approximate solutions. We will discuss the definition and approximation properties of a new family of GPWs.

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MS28

Spoof Plasmons and Double Negative Behavior in the Microwave Regime

We apply an asymptotic analysis to show that corrugated wave guides can be approximated by smooth cylindrical wave guides with an effective metamaterial surface impedance. We show that this approximation is in force when the period of the corrugations is subwavelength. Here the metamaterial delivers an effective anisotropic surface impedance and imparts novel dispersive effects on signals traveling inside the wave guide. These properties shown to arise from subwavelength resonances of the axial electric field component inside the perfectly conducting corrugations. Electric field resonances arising at microwave frequencies are known as spoof plasmons. True plasmon resonances arise from dielectric properties of noble metals at optical frequencies. For sufficiently deep corrugations, the metamaterial wave guide predicts backward wave propagation at microwave frequencies.

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MS28

High-Order Perturbation of Surfaces Algorithms for the Simulation of Localized Surface Plasmon Resonances in Graphene Nanotubes

The plasmonics of two–dimensional materials, such as graphene, has became an important field over the past decade. The active tunability of graphene via electrical gating or chemical doping has generated a great deal of excitement among engineers seeking sensing devices. Consequently there is significant demand for robust and highly accurate computational capabilities which can simulate such materials. The class of High–Order Perturbation of Surfaces methods have proven to be particularly appropriate for this purpose. In this talk we describe our recent efforts to utilize both Dirichlet–Neumann Operators and Impedance–Impedance Operators in these schemes. In addition, we present detailed numerical results which not only validate our simulations using the Method of Manufactured Solutions, but we also describe Localized Surface Plasmon Resonances in graphene nanotubes enclosing rodshaped dielectric materials.

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MS28

Hybridization of Singular Plasmons via Transformation Optics

Surface plasmons offer great opportunities to guide and manipulate light on the nanoscale. In the design of novel plasmonic devices, a central theme is to clarify the intricate relationship between the resonance spectrum and the geometry of the nanostructure. The design becomes quite challenging when the desired spectrum is highly complex. In this talk, we discuss a new theoretical model for surface plasmons of interacting nanoparticles to greatly reduce the complexity of the design problem. Our model is developed by combining plasmon hybridization theory with transformation optics, which yields an efficient way of simultaneously controlling both global and local features of the spectrum. As an application, we propose a design of metasurface whose absorption spectrum can be controlled over a large class of complex patterns through only a few geometric parameters in an intuitive way. Our approach provides fundamental tools for the effective design of plasmonic metamaterials with on-demand functionality. This talk is based on joint works with Habib Ammari (ETHZ).

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MS29

Super-Parameterized Boltzmann Equation for Sea Ice Modeling

We devise a super-parameterized sea ice model that captures dynamics at multiple scales. Sea ice contains many ice floes whose macro-scale behavior is driven by oceanic/atmospheric currents and floe-floe interaction. There is no characteristic floe size and accurately modeling dynamics requires a multi-scale approach. Our two-tiered model couples basin-scale conservation equations with small-scale particle methods. Unlike many sea ice models, we do not average quantities of interest (e.g., mass/momentum) over a representative volume. Instead, we explicitly model small-scale dynamics using the Boltzmann equation, which evolves a probability distribution over position and velocity. In practice, existing numerical methods are computationally intractable when modeling Arctic basin scale dynamics. We decompose the density function into a mass density that models how ice is distributed in the spatial domain and a velocity density that models the small-scale variation in velocity at a given location. The mass density and expected velocity evolve according to conservation equations. However, the flux term depends on expectations with respect to the velocity density at each spatial point. We use particle methods to simulate the conditional density at key locations and make each particle method independent using a change of variables that defines small-scale coordinates. We model small-scale ice dynamics (e.g., collision) in this transformed domain.

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MS29

Lagrangian Data Assimilation and Uncertainty Quantification for Sea Ice Floes with Efficient Superfloe Parameterization

Particle-based sea ice floe simulations are slow especially when the number of floes is large. We present a small-floe parameterization method to speed up the simulation by reducing the number of floes while maintaining the key features of the physics. In particular, we group the small floes that are close to each other into superfloes. Viewing each floe as a particle, the idea is similar to the coarsening process in the smoothed particle hydrodynamics method. The sizes, thickness, masses, and velocities of the superfloes are determined by conserving the sea ice concentration, mass, and momentum. We show that in a stochastic sense, the main features of the original simulations are well-maintained when using the floe-number-reduced simulation. As an application, we apply the parameterized superfloes to data assimilation with the purpose of assimilating the ocean current Fourier modes. For the purpose of simple tests, we adopt the widely-used ensemble adjustment Kalman filter (EAKF) for data assimilation. Various numerical experiments are presented to demonstrate the performance.

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MS29

Quantifying the Skill and Bias of Arctic Sea Ice Simulations

Benchmarking of sea ice simulations in coupled earth system models (ESMs) is now often carefully targeted toward specific polar physics and biogeochemistry and the associated coupling across sea ice, atmosphere and ocean. This talk addresses one aspect of benchmarking sea ice simulations using altimetric satellite emulators, which convert statistical distributions of sea ice thickness to synthesized ice freeboard as seen by laser altimeters aboard ICESat and ICESat-2. Freeboard emulation in earth system models can be approached using simple mathematical operators to convert between sub-grid scale parameterizations and the freeboard measured along 91-day repeat-orbit ground tracks of the aforementioned satellites. This provides an estimate of modeled ice and snow thickness accuracy, often adequate for many applications. However, more sophisticated operators that are aware of the scale of model grid cells and of the laser footprint can be constructed using variational techniques, and this talk focuses on this more advanced benchmarking method for the polar components of ESMs. We introduce the theory behind variational emulation, and demonstrate its capability using the Energy Exascale Earth System Model (E3SM) and Community Earth System Model (CESM). We also discuss simplified methods that may be applied post-factum to existing Coupled Model Intercomparison Project (CMIP) output, and relative accuracy in results that do not use the variational method.

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MS29

Discrete Element Simulations of Sea Ice Dynamics in the Nares Strait

Data-driven particle methods can provide detailed descriptions of sea ice dynamics that explicitly model fracture and discontinuities in the ice, which are difficult to capture with typical continuum approaches. We use the ParticLS software library to develop discrete element method (DEM) simulations of sea ice in the Nares Strait between Ellesmere Island and Greenland that are initialized from and driven by observed data. We model the sea ice as a collection of discrete rigid particles that are initially bonded together into floes. Ice fracture and lead formation are determined based on the local stress state around each particle. This allows us to model the ice as a continuous material while at the same time allowing it to fracture into smaller pieces that can then interact with each other as discrete bodies. In addition to modeling the dynamic sea ice patterns in the Nares Strait (arching, lead formation), our model provides a natural way to combine numerical simulations with observations. We generate realistic particle configurations by discretizing the ice extent in MODIS satellite imagery into polygonal floes, and then force the particles with wind and ocean data. We also investigate methods for validating regional-scale simulations, by quantitatively comparing model outputs to remote sensing measurements of the ice, which provides a rigorous approach for determining how well the model captures the dynamics observed in nature.

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MS30

Portfolio Liquidation Games with Self-Exciting Order Flow

We analyze novel portfolio liquidation games with self-exciting order flow. Both the N-player game and the mean-field game are considered. We assume that players' trading activities have an impact on the dynamics of future market order arrivals thereby generating an additional transient price impact. Given the strategies of her competitors each player solves a mean-field control problem. We characterize open-loop Nash equilibria in both games in terms of a novel mean-field FBSDE system with unknown terminal condition. Under a weak interaction condition we prove that the FBSDE systems have unique solutions. Using a novel sufficient maximum principle that does not require convexity of the cost function we finally prove that the solution of the FBSDE systems do indeed provide existence of open-loop Nash equilibria.

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MS30

A Finite Agent Equilibrium and Its Strong Convergence to the Mean-Field

We study the problem of equilibrium price formation in an incomplete securities market. Each financial firm (agent) tries to minimize its cost via continuous-time trading with a securities exchange while facing the systemic and idiosyncratic noises as well as the stochastic order-flows from its over-the-counter clients. We first construct a market clearing equilibrium among finite number of heterogeneous agents by a coupled system of forward-backward stochastic differential equations (FBSDEs), and then show its strong convergence to a certain FBSDE of conditional McKean-Vlasov type in the homogeneous large population limit. In particular, we provide a stability estimate between the market clearing price for the heterogeneous agents and that for the mean-field limit.

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MS30

Stochastic Differential Games on Random Directed Networks

We consider stochastic differential games on random directed networks with mean-field interactions, where the network of countably many players is formulated randomly in the beginning and each player in the network attempts to minimize the expected cost with a finite time horizon. Here, the cost function is determined by the network. Under the setup of the linear quadratic stochastic game with directed chain graph, we solve explicitly for an open-loop

Nash equilibrium for the system and we find that the dynamics under the equilibrium is an infinite-dimensional Gaussian process associated with a Catalan Markov chain. We extend it to the random directed tree structure and discuss convergence results.

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MS30

Human-Machine Interaction Models and Stochastic Optimization

I will introduce a model of human-machine interaction (HMI) in portfolio choice (robo-advising). Modeling difficulties stem from the limited ability to quantify the humans risk preferences and describe their evolution, but also from the fact that the stochastic environment, in which the machine optimizes, adapts to real-time incoming information that is exogenous to the human. Furthermore, the humans risk preferences and the machines states may evolve at different scales. This interaction creates an adaptive cooperative game with both asymmetric and incomplete information exchange between the two parties. As a result, challenging questions arise on, among others, how frequently the two parties should communicate, what information can the machine accurately detect, infer and predict, how the human reacts to exogenous events, how to improve the inter-linked reliability between the human and the machine, and others. Such HMI models give rise to new, non-standard optimization problems that combine adaptive stochastic control, stochastic differential games, optimal stopping, multi-scales and learning.

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MS32

Ciliary Motion Optimization of Axisymmetric Squirmers

This presentation focuses on optimizing the slip velocities on any given shape of an axisymmetric micro-swimmer suspended in a viscous fluid. The objective is to minimize the power loss to maintain a target swimming speed, or equivalently to maximize the efficiency of the micro-swimmer. Specifically, two types of slip velocities are considered: (1) Time-independent slip velocity and (2) Time-dependent, displacement-based slip velocity. We show that the time-independent optimization problem can be reduced to a simpler quadratic optimization problem, thanks to the linearity of the Stokes equations governing the fluid motion. This simplification bypasses the need for iterative optimization and enables a straightforward direct optimization. We also proposed a shape-based scalar metric that is predictive on whether the optimal swimmer of a given shape is a pusher or puller without the need of performing the optimization. In the displacement-based optimization, the slip velocity is induced by some periodic motion of the closely-packed ciliary tips. The forward problem is solved using a fast and accurate boundary integral method, and an adjoint-based method is adopted to compute the sensitivity of swimming efficiency. We found that, contrary to common beliefs, adding constraints to the ciliary length could lead to better swimming performance for some swimmer shapes.

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MS32

Nonlinear Dynamics of a Three-Layer Saffman-Taylor Problem

The three-layer Saffman-Taylor problem introduces two coupled moving interfaces separating the three fluids. In this talk, we present a weakly nonlinear analysis of this problem in a radial Hele-Shaw cell, and show that the morphologies of the emerging fingering patterns strongly depend on the initial thickness of the intermediate layer connecting the two interfaces. We then explore full nonlinear interfacial dynamics using a spectrally accurate boundary integral method. We quantify the nonlinear instability of both interfaces as the relevant physical parameters (e.g., viscosities and surface tensions) are varied and show that our nonlinear computations are in good agreement with the experimental observations and the weakly nonlinear analysis. Nonlinear simulations reveal that due to the existence of a second interface, the classical highly branched morphologies are replaced by less unstable structures in which finger tip-splitting and finger competition phenomena are evidently restrained as the initial annulus thickness is reduced.

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MS32

Shape Optimization of Peristaltic Pumps for Stokesian Flow using Boundary Integral Method

This work presents a new boundary integral approach for finding optimal shapes of peristaltic pumps transporting a viscous fluid or a rigid particle in Stokes flow. We consider shapes that minimize the rate of energy dissipation with a prescribed volume of fluid. When transporting a viscous fluid, we also constrain the mass flow rate; when transporting a rigid particle in Stokes flow, we constrain distance traversed by the particle over a set time period. Our approach relies on a recently developed fast and accurate boundary integral solver for simulating multiphase flows through periodic geometries of arbitrary shapes that completely avoid the issue of volume remeshing when updating the pump shape as the optimization proceeds. Formulas for computing the shape derivatives of the standard cost functionals and constraints are derived. In order to fully capitalize on the dimensionality reduction feature of the boundary integral methods, shape sensitivities must ideally involve evaluating the physical variables on the particle or pump boundaries only. We show that this can indeed be accomplished owing to the linearity of Stokes flow. We validate these analytic shape derivative formulas by comparing against finite-difference based gradients and present several examples showcasing optimal pump shapes under various constraints.

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MS32

Efficient Convergent Boundary Integral Methods for Slender Bodies

The dynamics of active and passive filaments in viscous fluids is frequently used as a model for many complex fluids in biological systems such as: microtubules which are involved in intracellular transport and cell division; flagella and cilia which aid in locomotion. The numerical simulation of such systems is generally based on slender-body theory which give asymptotic approximations of the solution. However, these methods are low-order and cannot enforce no-slip boundary conditions to high-accuracy, uniformly over the boundary. Boundary-integral equation methods which completely resolve the fiber surface have so far been impractical due to the prohibitive cost of current layer-potential quadratures for such high aspect-ratio geometries. In this talk, we will present new quadrature schemes which make such computations possible and present numerical results to show the efficiency of our method.

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MS33

An Eulerian-Lagrangian Finite Volume Method for Solving Nonlinear Transport Equations

There are two traditional approaches to numerically solving hyperbolic conservation laws: (1) a Lagrangian approach following particles along characteristics and (2) an Eulerian approach fixing a (uniform) spatial grid by discretizing the PDE in space. Lagrangian-based methods do not have a Courant-Friedrichs-Lewy (CFL) condition, but can require a remeshing step. Whereas, Eulerian-based methods can take advantage of high spatial resolution methods (e.g., weighted essentially nonoscillatory (WENO)) to control spurious oscillations, but require a CFL condition that forces a small time step. Eulerian-Lagrangian methods combine both frameworks by following approximate characteristics for a relaxed CFL condition, while still working on a fixed grid and taking advantage of high-resolution techniques. We introduce a new Eulerian-Lagrangian finite volume method that can be applied to both linear and nonlinear conservation laws.

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MS33

The Difference Potentials Method for Elliptic and Parabolic PDEs

Partial differential equations (PDEs) naturally arise in mathematical models from biology, engineering, medicine, and science. As analytical solutions of PDEs are typically unavailable, numerical methods for PDE are an important complement to modeling. This presentation will discuss the Difference Potentials Method (DPM), first developed by Viktor Ryabenkii, for the numerical approximation of elliptic and parabolic PDEs. We will show that the DPM leads to numerical schemes that are both highly accurate and computationally efficient. Time permitting, we will also discuss current research. This presentation will be for a general applied maths audience.

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MS34

Filtering Methods for Data Assimilation in Cardiovascular Simulation

A major challenge in constructing three-dimensional patient specific hemodynamic models is the calibration of model parameters to match patient data on flow, pressure, wall motion, etc. acquired in the clinic. Current workflows are manual and time-consuming. This work presents a flexible computational framework for model parameter estimation in cardiovascular flows that relies on the following fundamental contributions. i) A Reduced-Order Unscented Kalman Filter (ROUKF) model for data assimilation for wall material and simple lumped parameter network (LPN) boundary condition model parameters. ii) A constrained least squares augmentation (ROUKF-CLS) for more complex LPNs. iii) A "Netlist' implementation, supporting easy filtering of parameters in such complex LPNs. The ROUKF algorithm is demonstrated using non-invasive patient-specific data on anatomy, flow and pressure from a healthy volunteer. The ROUKF-CLS algorithm is demonstrated using synthetic data on a coronary LPN. The methods described in this paper have been implemented as part of the CRIMSON hemodynamics software package.

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MS34

Large-Scale Bathymetry Prediction using Deep Learning Approaches

The high cost and complex logistics of using ship-based surveys for bathymetry, i.e., depth imaging, have encouraged the use of various types of indirect measurements such as surface velocity from unmanned aerial vehicles. However, estimating high resolution bathymetry needed for hydrological and coastal applications from indirect measurements is usually an ill-posed inverse problem and can be computationally challenging as most of the inversion techniques require iterative calls to complex forward models to compute Jacobians and subsequent inversion of relatively large matrices. In this talk, we use a deep learning approach to accelerate bathymetry estimation for potential real-time waterbody depth imaging and subsequent forecast. Reduced order models of the shallow water equations are constructed on a nonlinear manifold of low dimensionality through variational encoders and the estimation with uncertainty quantification is performed on the low dimensional latent space in a Bayesian setting. Combined with automatic differentiation and stochastic Newton-type MCMC methods, we show that these proposed neural nets can perform the inversion operation much faster than traditional inversion methods. The improvement and performance of these methodologies are illustrated by applying them to riverine depth imaging problems.

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MS34

Quantifying and Mitigating Measurement Errors in Quantum Computing

Various noise models have been developed in quantum computing study to describe the propagation and effect of the noise from imperfect implementation of hardware. We infer such parameters using Bayesian approaches, and implement this method to study the gate and measurement error. By characterising the device errors in this way, we further improve error filters accordingly. Experiments conducted on IBMs quantum computing devices suggest that our approach provides more accurate error mitigation results than existing error-mitigation techniques, in which error rates are estimated as deterministic values.

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MS34

Improving Inverse Problem with Data Completion

Inverse problems are ubiquitous in the fabric of modern life, where we can find applications ranging from telecommunications to medical imaging. In the context of the latter inverse problems usually takes the form of estimating the properties inside the human body from measurement at its surface. In this context there usually exists a trade-off between the quality of the reconstruction and the cost of obtaining the data. Thus one seeks to obtain the best reconstruction quality with the smallest amount of data possible. In this talk, we tackle this issue by generating new artificial, or fake, data that is compatible with the physics of the problem and use it to feed optimization-based inversion algorithms. In particular, we exploit the low-rank structure of the data, to augment it using data-driven techniques in a hierarchical fashion. We will present the analytical and data-driven technique and their rationale. We will present some synthetic examples, showcasing the ability to complete unseen data, and improve the quality of the reconstruction.

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MS35

Influence of Noise Generation Techniques on the Modeling of Laser Beam Propagation in Turbulent Atmosphere based on Random Screens Approach

We considered two different approaches to noise screens generation for modeling of laser beam propagation in turbulent atmosphere. Specifically, we studied influence of these random noise generation techniques on the resulting pair correlation function of density in the screen. Also we study influence of the resulting noise fields on the integral characteristics of propagating beams and compared them with previously derived theoretical results. Influence of the resolution of the screen on these results was investigated as well.

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MS35

Motion of Singularities and Short Branch Cuts in Surface Dynamics

A potential motion of ideal incompressible fluid with a free surface and infinite depth is considered in two-dimensional geometry. A time-dependent conformal mapping of the lower complex half-plane of the auxiliary complex variable w into the area filled with fluid is performed with the real line of w mapped into the free fluid's surface. The fluid dynamics is fully characterized by the motion of the complex singularities in w plane. We consider the short branch cut approximation of the dynamics with the small parameter being the ratio of the length of the branch cut to the distance between its center and the real line of w. Fluid dynamics is reduced to the complex Hopf equation for the complex velocity coupled with the complex transport equation for the conformal mapping. These equations are fully integrable by characteristics producing the infinite family of solutions, including the pairs of moving square root branch points. The solutions are compared with the simulations of the full Eulerian dynamics giving excellent agreement. We consider the dynamics of singularities and finite time blowup of Constantin-Lax-Majda equation which corresponds to non-potential effective motion of non-viscous fluid with competing convection and vorticity stretching terms. A family of exact solutions is found together with the different types of complex singularities approaching the real line in finite times. References: arXiv:2003.05085, arXiv:2010.01201

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MS35

A Hybrid Boundary Integral Method for Two-Phase Flow with Soluble Surfactant

We present an accurate and efficient numerical method to simulate the deformation of drops and bubbles in Stokes flow with soluble surfactant. The method builds on a recent hybrid or multiscale numerical method developed by the authors to address difficulties in the numerical computation of fluid interfaces with soluble surfactant in the physically representative large Peclet number limit. In this limit, a thin transition layer develops near the interface in which physical quantities rapidly vary, yet must be well resolved for accurate computation of the interface dynamics. The hybrid method uses the slenderness of the layer to incorporate a separate analytical reduction of the layers dynamics into a novel boundary integral formulation of the interfacial free boundary problem. Up to now, the hybrid method has been designed to treat systems of drops and bubbles for which the bulk concentration of soluble surfactant is present in the exterior fluid alone. Although this is a good assumption in some applications, there are situations in which surfactant is present in the interior fluid, or can transfer between the exterior and interior fluid via transport through the combined interface-transition layer structure. In this talk we present a method that removes this limitation.

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MS35

Stability of Periodic Standing Waves in the Derivative Nls Equation

We consider the periodic standing waves of the derivative nonlinear Schrödinger equation. We begin by classifying all periodic standing waves in terms of eigenvalues of the Kaup-Newell spectral problem, and then study the stability of some of the solutions using the numerical Hill's method. We demonstrate that all of the "nontrivial phase" solutions, except for one class, are spectrally unstable.

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MS36

A Biomimetic Approach to Sensing with Waves

The aim of our work is to establish the mathematical foundations for the design of biomimetic sensing devices. Such devices aim to take advantage of nature's remarkable ability to devise innovative solutions to challenging problems. In this talk, we explore these ideas through a case study on human hearing. Using boundary integrals and asymptotic techniques, we design a subwavelength acoustic metamaterial that mimics the performance of the cochlea. Building on this, we are then able to use our mathematical framework explore theories of cochlear amplification and also to deduce related signal processing algorithms.

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MS36

Asymptotic Posterior Normality for the Bayesian Inversion of the Non-Abelian X-Ray Transform on Simple Surfaces

The non-abelian X-ray transform is a non-linear integral geometric operator whose inversion has applications to Polarimetric Neutron Tomography. The latter is an imaging modality which aims at recovering the magnetic field inside a medium from spin-in to spin-out measurements of neutron beams. This transform, while being non-linear, enjoys rather precise answers to questions of injectivity, stability and mapping properties, which in turn help a successful analysis of the following statistical question: find a statistically reliable strategy to reconstruct a matrix field from its noisy non-abelian X-ray transform. In short: in the Bayesian framework and under a certain (flexible) choice of prior, the posterior mean gives a consistent estimator, and the posterior distribution becomes locally asymptotically normal (a Bernstein-von Mises type of theorem). In this talk, we will discuss the results and some elements of proof.

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MS36

A Dimension-Reduction Approach to Cross-Correlation Based Imaging

We are interested in recovering a sparse signal from intensity-only measurements. In contrast to the case of known phases, the unknown is now a matrix formed by the cross correlation of the unknown signal. Hence, the bottleneck for inversion is the number of unknowns that grows quadratically. We propose to reduce the dimensionality of the problem by recovering only a part of the matrix of the cross-correlations. I will consider 2 cases. In the first case we use diversity of illuminations and the the diagonal of the unknown matrix to obtain a stable image. In the second case we use only one illumination, and exploit the symmetries of the imaging matrix to reduce the inversion to the turnpike problem. The turnpike problem is a classic inverse problem of recovering a set of points from the set of their pairwise differences Both approaches lead to linear number of unknowns.

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MS36

Stable Reconstruction of Simple Riemannian Manifolds from Unknown Interior Sources

Consider the geometric inverse problem: There is a set of delta-sources in spacetime that emit waves travelling at unit speed. If we know all the arrival times at the boundary cylinder of the spacetime, can we reconstruct the space, a Riemannian manifold with boundary? With a finite set of sources we can only hope to get an approximate reconstruction, and we indeed provide a discrete metric approximation to the manifold with explicit data-driven error bounds when the manifold is simple. This is the geometrization of a seismological inverse problem where we measure the arrival times on the surface of waves from an unknown number of unknown interior microseismic events at unknown times. The closeness of two metric spaces with a marked boundary is measured by a labeled Gromov–Hausdorff distance. If measurements are done for infinite time and spatially dense sources, our construction produces the true Riemannian manifold and the finite-time approximations converge to it in the metric sense. This talk is based on a joint work with Maarten V. de Hoop, Joonas Ilmavirta and Matti Lassas

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MS38

Qualitative Properties of Certain FSI PDE Models

In this study, we consider a linearized compressible flow structure interaction PDE model for which the interaction interface is under the effect of material derivative term. While the linearization takes place around a constant pressure and density components in structure equation, the flow linearization is taken with respect to a non-zero, fixed, variable ambient vector field. This process produces extra convective derivative and material derivative terms which causes the coupled system to be nondissipative. We analyze the long time dynamics in the sense of asymptotic (strong) stability in an invariant subspace (one dimensional less) of the entire state space where the continuous semigroup is uniformly bounded. For this, we appeal to the pointwise resolvent condition introduced by Chill and Tomilov which avoids many technical complexity and provides a very clean, short and easy-to-follow proof.

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MS38

Boundary Control for Optimal Mixing: from Open-Loop to Closed-Loop

This talk focuses on the control problems for optimal mixing via flow advection in an open bounded and connected domain. Both open- and closed-loop control designs will be discussed. Numerical examples will be presented to demonstrate the ideas.

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MS38

Weak and Strong Attractors in Structural Acoustic Kirchhoff Boussinesq Interactions with Boundary Damping

We consider a structural-acoustic problem in dimension 3, in which the structural wall is modeled by a 2D Kirchhoff-Boussinesq plate and acoustic medium is subject to boundary damping. For this model we study existence of a continuous nonlinear semigroup along with long time behavior associated with the model and finite energy space. It will be shown that strong/weak continuity of the semigroups and strong/weak attractiveness depend on the support of the boundary damping. The difficulty is related to supercritical nonlinearity exhibited by the plate along with the compromised boundary regularity of the acoustic waves. Compensated compactness methods along with a hidden boundary regularity of hyperbolic traces are exploited in order to establish weak (resp. strong) generation of a nonlinear semigroup subjected to feedback forces placed on the boundary of the acoustic medium. Accordingly, weak/strong attractors for the model will be constructed by relying on recent estimates generated by the quasistability theory.

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MS38

Simultaneous Controllability of Two Parabolic Equations

In this talk, we present some results on the simultaneous null controllability of two (uncoupled) parabolic equations. That is, with the same input function we look for conditions on the parameters on each one to control simultaneously both equations. Probably the first result in this direction is due to Russell in his study of the boundary controllability of Maxwell's equations. In his work, he deals with the simultaneous controllability of two uncoupled wave equations with different boundary conditions. After this seminal paper, there is intensive research on related subjects but treating hyperbolic equations. See the interesting work due to Tbou on simultaneous control of semilinear wave equations and the references in it, for a complete panorama on the subject.

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MS39

Deep Neural Network Expression of Posterior Expectations in Bayesian PDE Inversion

For Bayesian inverse problems with input-to-response maps given by well-posed partial differential equations (PDEs) and subject to uncertain parametric or function space input, we establish (under rather weak conditions on the forward', input-to-response maps) the parametric holomorphy of the data-to-QoI map relating observation data δ to the Bayesian estimate for an unknown quantity of interest (QoI). We prove exponential expression rate bounds for this data-to-QoI map by deep neural networks with rectified linear unit (ReLU) activation function, which are uniform with respect to the data δ taking values in a compact subset of $\mathbb{R}^K$. We propose an efficient, deterministic algorithm for constructing exponentially convergent deep neural network approximations of multivariate, analytic maps $f : [-1, 1]^K \to \mathbb{R}$. This construction is applicable to the data-to-QoI map.

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MS39

Overcoming the Curse of Dimensionality: from Nonlinear Monte Carlo to Deep Learning

Partial differential equations (PDEs) are among the most universal tools used in modelling problems in nature and man-made complex systems. For example, Hamiltonian-Jacobi-Bellman PDEs are employed in operations research to describe optimal control problems and Black-Scholes-type PDEs are employed in state-of-the-art pricing and hedging models for financial derivatives. The PDEs appearing in such models are often high-dimensional. Such PDEs can typically not be solved explicitly and it is one of the most challenging tasks in applied mathematics to develop approximation algorithms which are able to approximatively compute solutions of high-dimensional PDEs. Most of the approximation algorithms for PDEs in the literature suffer from the so-called "curse of dimensionality" in the sense that the number of required computational operations of the approximation algorithm to achieve a given approximation accuracy grows exponentially in the dimension of the considered PDE. With such algorithms it is impossible to approximatively compute solutions of high-dimensional PDEs even when the fastest currently available computers are used. In this talk we prove that suitable deep neural network approximations do indeed overcome the curse of dimensionality in the case of a general class of semilinear parabolic PDEs and we thereby prove that a general semilinear parabolic PDE can be solved approximatively without the curse of dimensionality.

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MS39

Neural Operator: Learning Maps Between Function Spaces

The classical development of neural networks has primarily focused on learning mappings between finite dimensional Euclidean spaces or finite sets. We propose to generalize neural networks so that they can learn operators mapping between infinite dimensional function spaces. We formulate the approximation of operators by composition of a class of linear integral operators and nonlinear activation functions, so that the composed operator can approximate complex nonlinear operators. We propose four formulations of the integral operators: graph-based operators, low-rank operators, multipole graph-based operators, and Fourier operators. The proposed neural operators are resolution-invariant: they share the same network parameters between different discretizations and they can do zero-shot super-resolutions. We perform experiments on temporal dynamics and chaotic systems. The proposed models show superior performance compared to existing machine learning based methodologies. Meanwhile, they are several magnitudes faster compared to conventional PDE solvers.

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MS39

Optimal Experimental Design for Large-Scale Bayesian Inverse Problem with Deep Neural Network Surrogate

In this talk, we present a deep learning framework for optimal experimental design (OED). OED plays an important role in optimally acquiring observation data to reduce parameter uncertainty by Bayesian inference. It is formulated as an optimization problem that requires numerous evaluation of suitable optimal criterion, for which an inner

Bayesian inverse problem have to be solved. This is computationally prohibitive if the forward model (e.g. large-scale PDE with high-dimensional parameters) is expensive to solve. To reduce the computational cost, we develop a deep learning framework that constructs a projected neural network (PNN) to learn the parameter-to-observable map and its Jacobian. We use the PNN as a surrogate to accelerate the evaluation of the optimal criterion and the OED optimization. Numerical results are presented to demonstrate the accuracy and efficiency of this framework.

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MS40

Phase Models of Sea Ice Fracture

Fractures impact sea ice dynamics across a wide range of spatial scales: basin-scale leads enhance atmosphere-ocean heat transfer and polar albedo; fractures within ice connect air and brine pockets to form brine channels. Modeling realistic break up of a single ice floe requires expensive, high resolution measurements. Elastic properties of a floe vary with porosity, temperature, age and thickness. Sharp changes in elastic deformation and corners localized stress and nucleate fractures. We are developing a framework for efficiently generating simulated data banks of fractured floes for a large number of realizable parameters. Phase-field models employ a continuous order parameter to distinguish between broken and unbroken regions. Using these models, we insert realizations of physical floe parameters and geometries to produce a bank of fracture profiles.

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MS40

Modeling Lead Development in Continuous Sea Ice Floes with a Hybrid Peridynamic Discrete Element Method

The Arctic has undergone significant changes in recent decades due to climate change, with substantial reductions in sea ice extent and multiyear ice, leading to thinner ice that is susceptible to breakup. This so called "New Arctic" presents many challenges including, but not limited to, accurately modeling sea ice dynamics, lead (crack) development, and ridge formation (sea ice floe collision). Particle methods, such as the discrete element method (DEM), can provide detailed descriptions of sea ice dynamics that explicitly model fracture and ridging, which can be difficult with typical continuum sea ice modeling approaches. However, large sea ice floes can deform and break up under external forcing, which presents challenges for a DEM to simulate these important dynamics accurately. In this talk, we present our current efforts in extending sea ice DEM formulations to model continuous floe mechanics with a novel sea ice peridynamic-DEM hybrid model. We will present results on idealized tests that examine the ability of the model to predict effective continuous sea ice properties including effective stress and strength. Lastly, we discuss results from simulations of sea ice dynamics through the Nares Strait. We compare our simulation results to optical satellite imagery and discuss predictive capability.

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MS40

Data-Driven Operator-Theoretic Prediction and Dynamics of Sea Ice in the Baltic Sea

We present a new data-driven for prediction scheme, combining kernel methods for machine learning and operator-theoretic ergodic theory. This method, called kernel analog forecasting (KAF), is a generalization of Lorenz's analog forecasting approach that rigorously approximates the conditional expectation of observables under partially observed, nonlinear dynamics, while also providing useful uncertainty quantification through estimates of conditional variance and conditional probability. We perform forecasting of sea ice in the Baltic Sea. Furthermore, we examine prediction skill and its correspondence with eigenfunctions of Koopman operators acting across a range of timescales.

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MS41

A Mean-Field Game Approach to Equilibrium Pricing in Solar Renewable Energy Certificate Markets

Solar Renewable Energy Certificate (SREC) markets are a market-based system that incentivizes solar energy generation. A regulatory body imposes a lower bound on the amount of energy each regulated firm must generate via solar means, providing them with a tradeable certificate for each MWh generated. Firms seek to navigate the market optimally by modulating their SREC generation and trading rates. As such, the SREC market can be viewed as a stochastic game, where agents interact through the SREC price. We study this stochastic game by solving the mean-field game (MFG) limit with sub-populations of heterogeneous agents. Market participants optimize costs accounting for trading frictions, cost of generation, non-linear non-compliance costs, and generation uncertainty. Moreover, we endogenize SREC price through market clearing. We characterize firms' optimal controls as the solution of

McKean-Vlasov (MV) FBSDEs and determine the equilibrium SREC price. We establish the existence and uniqueness of a solution to this MV-FBSDE, and prove that the MFG strategies form an ϵ-Nash equilibrium for the finite player game. Finally, we develop a numerical scheme for solving the MV-FBSDEs and conduct a simulation study.

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MS41

Solving Mean-Field PDEs with Symmetric Neural Networks

We propose numerical methods for solving non-linear partial differential equations (PDEs) in the Wasserstein space of probability measures, which arise notably in the optimal control of McKean-Vlasov dynamics. The method relies first on the approximation of the PDE in infinite dimension by a backward stochastic differential equation (BSDE) with a forward system of N interacting particles. We provide the rate of convergence of this finite-dimensional approximation for the solution to the PDE and its L-derivative. Next, by exploiting the symmetry of the particles system, we design a machine learning algorithm based on certain types of neural networks, named PointNet and DeepSet, for computing simultaneously the pair solution to the BSDE by backward induction through sequential minimization of loss functions. We illustrate the efficiency of the PointNet/DeepSet networks compared to classical feedforward ones, and provide some numerical results of our algorithm for the examples of a mean-field systemic risk and a mean-variance problem.

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MS41

The Entry and Exit Game in the Electricity Markets: A Mean-Field Game Approach

We develop a model for the industry dynamics in the electricity market, based on mean-field games of optimal stopping. In our model, there are two types of agents: the renewable producers and the conventional producers. The renewable producers choose the optimal moment to build new renewable plants, and the conventional producers choose the optimal moment to exit the market. The agents interact through the market price, determined by matching the aggregate supply of the two types of producers with an exogenous demand function. Using a relaxed formulation of optimal stopping mean-field games, we prove the existence of a Nash equilibrium and the uniqueness of the equilibrium price process. An empirical example, inspired by the UK electricity market is presented. The example shows that while renewable subsidies clearly lead to higher renewable penetration, this may entail a cost to the consumer in terms of higher peakload prices. In order to avoid rising prices, the renewable subsidies must be combined with mechanisms ensuring that sufficient conventional capacity remains in place to meet the energy demand during peak periods.

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MS41

Covid-19: A Data-Driven Mean-Field-Type Game Perspective

In this talk, a class of mean-field-type games with discrete-continuous state spaces will be presented. We establish Bellman systems which provide sufficiency conditions for mean-field-type equilibria in state-and-mean-field-type feedback form. We then derive a master adjoint system (MASS). The methodology is shown to be flexible enough to capture multi-class interaction in epidemic propagation in which multiple authorities and firms are risk-aware atomic decision-makers and individuals are risk-aware non-atomic decision-makers. Based on MASS, we present a data-driven modelling and analytics for mitigating Coronavirus Disease 2019 (COVID-19). The model integrates vaccination, untested cases, age-structure, decision-making, gender, pre-existing health conditions, location, testing capacity, hospital capacity, and a mobility map of local areas, including in-cities, inter-cities, and internationally. It is shown that the data-driven model can capture most of the reported data on COVID-19 on confirmed cases, deaths, recovered, number of testing and number of active cases in 100+ countries. The model also reports non-Gaussian, and non-exponential properties in 35+ countries.

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MS42

High-Order Bound-Preserving Discontinuous Galerkin Methods for Multiphase Flow

We consider the high-order bound-preserving local discontinuous Galerkin method for the simulation of incompressible and immiscible two-phase flow in porous media with capillary pressure. Mathematical model of two-phase flow in porous media is a couple system of time-dependent nonlinear PDEs which include the Darcys law, the equation of conservation of mass for each phase, the constraint of the saturations of phases, and the equation of capillary pressure which depends on the wetting saturation. The important physical features of the saturations of phases is their boundedness between 0 and 1. Failure of bound-preserving of saturations may cause blow-ups of the numerical algorithm. We propose high-order bound-preserving local discontinuous Galerkin method to keep this important physical feature. Numerical examples are given to demonstrate the high-order accuracy and bound-preserving property of the numerical technique.

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MS42

Coupled Fluid Flow and Geomechanical Modeling for Understanding the Mechanism of Shear Dilation in Bedding Layers Induced by Hydraulic Fracturing

In this paper, a coupled fluid flow and geo-mechanical model was developed to better understand the physical process of bedding layer shear dilation and its impact on hydraulic fracture propagation and height growth. To accurately capture the shear slippage and propagation of the bedding layers induced by the hydraulic fracture, we applied a higher order displacement discontinuity method (HDDM), which outperforms the constant displacement discontinuity method (DDM) in accuracy but maintains the same computational efficiency. Different from the hydraulic fracture propagation, the shear slippage propagation of a bedding layer starts with the fracturing fluid leaking into the bedding layer, which elevates the fluid pressure and therefore decreases the resistive shear strength induced by the effective normal stress. When the shear failure criterion is satisfied, shear failure occurs and the shear dilation is activated. The shear dilation increases the permeability of the bedding layer and speeds up the fluid leak off, which results in a positive reinforcement of the shear propagation. This process is slowing down the hydraulic fracture height propagation due to fluid loss and conductivity enhancement in the bedding layer. Case studies show that the fluid viscosity, initial bedding layer width, and the maximum effective hydraulic aperture of the bedding layer have significant impacts on the shear dilation process.

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MS42

High-Order Bound-Preserving Finite Difference Methods for Miscible Displacements in Porous Media

In this paper, we develop high-order bound-preserving (BP) finite difference (FD) methods for the coupled system of compressible miscible displacements. We consider the problem with multi-component fluid mixture and the (volumetric) concentration of the jth component, c_j, should be between 0 and 1. It is well known that c_j does not satisfy a maximum-principle. Hence most of the existing BP techniques cannot be applied directly. The main idea in this paper is to construct the positivity-preserving techniques to all $c_j's$ and enforce $\sum_j c_j = 1$ simultaneously to obtain physically relevant approximations. By doing so, we have to treat the time derivative of the pressure dp/dt as a source in the concentration equation and choose suitable "consistent' numerical fluxes in the pressure and concentration equations. In order to develop high-order BP FD methods, we first construct a special discretization of the convection term, which yields the desired approximations of the source. Then we can find out the time step size that suitable for the BP technique and apply the flux limiters. Moreover, we will also construct a special algorithm for the diffusion term whose stencil is the same as that used for the convection term. Numerical experiments will be given to demonstrate the high-order accuracy and good performance of the numerical technique.

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MS42

An Integrated Equation-of-State Compositional Hydraulic Fracturing and Reservoir Simulator

We present an integrated Equation-of-State based compositional hydraulic fracturing and reservoir simulator. The goal of this research is to develop a general simulator that can simulate the lifecycle of wells, which includes hydraulic fracturing treatment using water-based or energized (gas, foam) fracturing fluid, post-frac shut-in and flowback, primary production, and fluid reinjection in a multiple well pad. This simulator fully couples the reservoir, fracture, and wellbore domains with multiple physics in each domain. The rock deformation, porous flow and temperature change in the reservoir domain, fluid and proppant transport in the fracture domain, and wellbore slurry flow and fluid/proppant distribution among clusters are fully coupled together and solved fully implicitly using the Newton-Raphson method. The phase behavior of hydrocarbon phases is modeled using Peng-Robinson Equation-of-state. The fracture propagation is modeled by mesh topology change and the propagation direction is evaluated using the stress intensity factors. This simulator has been fully parallelized using MPI and domain decomposition method and a speedup test has been performed using the Stempede2 supercomputer at Texas Advanced Computing Center. This simulator is validated against various problems with known analytical solutions. We show two applications of this simulator for lifecycle analysis in US unconventional oil reservoirs on frac-hits and CO2 fracturing.

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MS43

The Pole Dynamics of Soliton Solutions of the Focusing Nls Equation

The dynamics of the soliton solutions of the focusing Nonlinear Schrodinger equation is examined through the study of their poles in the complex x-plane. These poles are time dependent and their interactions in the x-plane provide a new way to understand soliton collisions. We limit our study to the case where the multi-soliton asymptotically approaches a linear superposition of single solutions. Thus breathers or resonant solitons are not yet considered.

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MS43

Self-Similar Evolution in Wave Turbulence and Nonequiliblium Bose-Einstein Condensation

Creation of turbulent states in Bose-Einstein condensates (BEC) has recently become a rapidly developing direction in experimental research. This is because of the versatility of the optical control and measurement techniques in BEC experiment which make it a perfect laboratory for studies of turbulence. BEC turbulence is a rich system posessing many key attributes of the classical and quantum turbulence and wave turbulence including randomly interacting dispersive waves, quantized vortices, forward and inverse cascades. In my talk I will overview the current state of art in the theory, numerical modeling and recent experiments in BEC turbulence. I will introduce the theory of wave turbulence (WT) that discribes some important features of BEC turbulence and non-equilibrium condensation. I will describe transitions from weak WT to strong turbulence dominated by a gas of strongly nonlinear quantized vortices, whose subsequent anihilations result in appearance of a coherent condensate state. I will describe remaining theoretical challenges in theoretical description of turbulent states where random waves and vortices coexist and interact, and will discuss proposals of novel experimental setups.

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MS43

Suppression of Turbulent Transport by Zonal Flows in Magnetized Plasmas

We introduce a new reduced fluid model to understand the abrupt change in the turbulent plasma dynamics which can take place at the edge of magnetic confinement fusion devices, with the spontaneous appearance of macroscopic, zero-frequency shear flows known as zonal flows. Our model is based on a modification of the well-known Hasegawa-Wakatani model [M. Wakatani and A. Hasegawa, Physics of Fluids 27(3), 611618 (1984); R. Numata, R. Ball, and R. L. Dewar, Physics of Plasmas 14(10), 102312 (2007)], with an improved treatment of the electron dynamics parallel to the magnetic field. In this talk, we will present the main properties of our model, discuss the role of boundary conditions, and if time permits, investigate effective strategies and algorithms for uncertainty quantification for that complex dynamical system.

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MS43

On Propagation of Pulses in Neurons

I will report on recent work with A. Talidou and A. Burchard in which we consider the FitzHugh-Nagumo equation extended to cylindrical surfaces. We show the existence of stable pulse-like solutions close to exact 1-dimensional pulses.

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MS44

Coupling Estimates for Stochastic Sampling Quality

We present algorithms to quantitatively assess the accuracy of stochastic samplers, particularly in cases where the analytic form of the invariant measure is unavailable. In many cases, the invariant measure of the numerical sampler, $\hat{\pi}$, is different from the true invariant measure π, and we give numerical schemes to quantitatively estimate the distance between the measures. This is done with a coupling method to estimate the contraction rate of the transition kernel, and we present extensions to cases with degenerate noise.

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MS44

Examining Diminishing Returns in Exhaustive Saddle Point Searches

In calculating the time evolution of an atomic system on diffusive timescales, off lattice kinetic Monte Carlo (OLKMC) can sometimes be used to overcome the limitations of Molecular Dynamics. OLKMC relies on the harmonic approximation to Transition State Theory, in which the rate of rare transitions from one energy minimum to a neighboring minimum scales exponentially with an energy barrier on the potential energy surface. This requires locating the index-1 saddle point, commonly referred to as a transition state, that separates two neighboring energy minima. In modeling the evolution of an atomic system, it is desirable to find all the relevant transitions surrounding the current minimum. Due to the large number of minima on the potential energy surface, exhaustively searching the landscape for these saddle points is a challenging task. In examining the particular case of isolated Lennard-Jones clusters of around 50 particles, we observe very slow convergence of the total number of saddle points found as a function of successful searches. We seek to understand this behavior by modeling the distribution of successful searches and sampling this distribution to create a stochastic process that mimics this behavior.

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MS44

Accurate and Efficient Splitting Methods for Dissipative Particle Dynamics

We study numerical methods for dissipative particle dynamics (DPD), which is a system of stochastic differential equations and a popular stochastic momentum-conserving thermostat for simulating complex hydrodynamic behavior at mesoscales. We propose a new splitting method that is able to substantially improve the accuracy and efficiency of DPD simulations in a wide range of the friction coefficients, particularly in the extremely large friction limit that corresponds to a fluid-like Schmidt number, a key issue in DPD. Various numerical experiments on both equilibrium and transport properties are performed to demonstrate the superiority of the newly proposed method over popular alternative schemes in the literature.

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MS44

A Splitting Method to Reduce MCMC Variance

We explore whether splitting and killing methods can improve the accuracy of Markov chain Monte Carlo (MCMC) estimates of rare event probabilities, and we make three contributions. First, we prove that "weighted ensemble" is the only splitting and killing method that provides asymptotically consistent estimates when combined with MCMC. Second, we prove a lower bound on the asymptotic variance of weighted ensemble's estimates. Third, we give a constructive proof and numerical examples to show that weighted ensemble can approach this optimal variance bound, in many cases reducing the variance of MCMC estimates by multiple orders of magnitude.

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MS45

Rogue Waves in Integrable and Non-Integrable Systems: Existence, Stability and Dynamics

This talk will focus on the formation of rogue waves in the nonlinear Schrödinger (NLS) equation and the Salerno model containing the integrable Ablowitz-Ladik (AL) and (non-integrable) discrete NLS (DNLS) models. We will first consider Gaussian wavepacket initial data for both the NLS and Salerno models, where novel spatio-temporal dynamics will be presented as the Gaussian's width changes. We will show that large amplitude excitations strongly reminiscent of the Peregrine soliton, (time-periodic) Kuznetsov-Ma (KM) breather or regular solitons appear to form. Then, we will focus on the existence, stability and dynamics of discrete Kuznetsov-Ma breathers in the Salerno model. We will explore the configuration space of KM breathers by varying the period of the solution and the homotopy parameter associated with the Salerno model (connecting the AL and DNLS models). We will show that on one hand, the KM breather in the AL model is not the only one solution since more KM solutions bearing oscillatory tails are shown to be present therein. On the other hand, and as per the DNLS model, novel KM breathers will be presented in this case. The results will be complemented by a discussing the stability of the solutions using Floquet theory and numerical simulations. More recent results on the DNLS equation will be presented too (if time permits) and open problems and questions will be discussed.

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MS45

An Integrable Two-Component Generalization of the Degasperis-Procesi Equation

We propose an integrable two-component generalization of the Degasperis-Procesi (DP) equation. We found that the Witten-Dijkgraaf-Verlinde-Verlinde (WDVV) equation can be reduced to a two-component DP equation. Based on this fact, we construct the Lax pair, the bi-Hamiltonian structure and conservation laws for this newly integrable coupled equation.

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MS45

Ist and Solitons for the Complex Coupled Short-Pulse Equation

We present the inverse scattering transform (IST) for the complex coupled short pulse equation (cSPE) on the line. Our work extends to the complex, coupled case the Riemann-Hilbert approach to the IST for the real, scalar short-pulse equation proposed by A. Boutet de Monvel and collaborators in 2017. One-soliton solutions are also investigated within the framework of the IST. The simplest soliton solutions, fundamental solitons, are found to be the natural vector generalization of scalar one-soliton solutions of the complex short-pulse equation. But in the coupled case one can also have more complicated, composite soliton solutions, corresponding to two fundamental solitons having the same amplitude and velocity but different carrier frequencies, as well as solutions that, while still corresponding to a minimal set of discrete eigenvalues, cannot be reduced to simple superposition of fundamental solitons. It is also found that the same constraints on the discrete eigenvalues that guarantee regular, smooth solutions also hold in the coupled case.

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MS45

Multicomponent Solitons in Atomic Bose-Einstein Condensates

In this talk, we will mention a number of recent developments on multi-component wave patterns in Bose-Einstein condensates. We will discuss various states in two-component systems including recently observed ones experimentally such as dark-bright and dark-antidark solitonic ones. Then we will extend consideration to three-component spinor settings and first discuss their ground state structure, and subsequently super-impose on the same parametric space the diagram of existence of different excited nonlinear wave states. We will also present further developments which go beyond the standard spinor model and towards the classical Manakov model, where an experimental connection with integrability becomes accessible. There, we will encounter dark-bright-bright soliton states and explore how their collisional properties follow predictions of polarization shifts made on the basis of the theory of integrable systems theory.

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MS46

Domains Without Dense Steklov Nodal Sets

This talk concerns the asymptotic geometric character of the nodal set of the eigenfunctions of the Steklov eigenvalue problem in two-dimensional domains. In particular results will be mentioned which establish the existence of a dense family $\mathcal{A}$ of simply-connected two-dimensional domains with analytic boundaries for each one of which the Steklov eigenfunction's nodal lines "are not dense at scale $1/j$". This result, which addresses a question put forth under "Open Problem 10" in Girouard and Polterovich, J. Spectr. Theory, 321-359 (2017), shows that, for domains in the class $\mathcal{A}$, the Steklov nodal sets have starkly different character than anticipated: they are not dense at any shrinking scale. A variety of numerical results, including surprising graphical manifestations of the non-dense nodal character, will also be presented. Work in collaboration with Jeffrey Galkowski.

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MS46

Application of the Feast Algorithm to Computing Fiber Modes

Most of the energy carried in optical fibers resides in a few transverse modes of the fiber. These transverse modes may be of the guided type, or the leaky type (with low losses). Due to the millions of wavelengths contained in a typical fiber length, the only feasible way to simulate complex nonlinear effects in fibers is by using simplified models. We use reduced-order models built using the transverse modes. For simple geometries, like the textbook step-index fiber, these modes can be analytically computed in closed form. However, for emerging microstructured fibers, they must be computed by numerically by solving an eigenproblem. In this talk we focus on the computation of leaky modes and loss factors. Using a frequency-dependent perfectly matched layer and a high-order finite element discretization, we arrive at a nonlinear eigenproblem. We solve this eigenproblem using a variant of the popular FEAST algorithm. We present the details involved in both the linear algebra as well as in the discretization.

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MS46

On Mixed Steklov Eigenvalue Problems

We present recent results on the spectra of mixed Steklov-Neumann problems for the Laplacian as well as the Helmholtz operator. Key to the work is a boundary integral discretization strategy, which we describe in detail.

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MS46

An Algorithm for Exploring Eigenvector Localization

It is well-known that domain geometry and "disorder" in the coefficients of a differential operator can give rise to localization (concentration of mass) of some eigenvectors in relatively small subdomains. A rich literature concerning such localization phenomena has developed over the past 60 years, and new mathematical insights into the underlying mechanisms driving localization have been provided over the last decade. Much more recently, a few numerical methods have been proposed for identifying likely regions of localization, and estimating eigenpairs (or just the eigenvalues) for which the eigenvector is localized in such a region. We propose a new method, which targets eigenvectors that are localized in a specified region R, incorporating a tolerance that quantifies how strongly concentrated the eigenvector must be within the region to be accepted as being "localized" there. Our approach is inspired by the work of Marletta on combating the effects of spectral polution when computing eigenvalues of an operator that are near its essential spectrum. Though the operators we consider have no essential spectrum, our approach similarly involves a complex shift of the operator, which is designed to highlight eigenpairs for which the eigenvector is localized in R within a given tolerance. We provide theory supporting our proposed approach, and numerical examples illustrating its performance. This is joint work with Robyn Reid.

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MS47

High-Resolution Remote Sensing Sea Ice Observations for Improved Prediction

Observations of Arctic sea ice reveal a negative and accelerating trend of end-of-summer extent, outpacing model projections, which suggests some sea ice processes are not well represented in models. In summer, snow atop the sea ice melts into ponds, decreasing surface albedo and contributing to the ice albedo feedback. Recent model sensitivity studies have shown that including melt pond (MP) parameters in sea ice forecasting end-of-summer ice predictions. In summer, abundant moisture due to extensive open water areas results in the formation of low-lying clouds that can obscure surface observations. MPs appear radiometrically similar to open water and leads, impeding disambiguation of these features. Thus, our understanding of MP processes is lacking at an Arctic-wide level. Scientists rely on predictive models to supplement the limited summer observations. We present new observational data from the ICESat-2 satellite that may be of interest to the modeling community. ICESat-2, launched by NASA in 2018, has demonstrated the ability to precisely (2 cm) measure sea ice height with along-track sampling of 0.7m. We present examples of high-resolution spring sea ice topography and freeboard that may be used for model initialization, and new observations of MPs that may be used for validation of summer sea ice forecasting. Our ICESat-2 results are complemented by extensive, high-resolution airborne observations of MPs collected by Operation IceBridge in July 2016 and 2017.

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MS47

Characterizing the Sea-Ice Floe Size Distribution Across a Range of Settings from High-Resolution Optical Satellite Imagery

The Arctic sea-ice floe size distribution (FSD) is a metric of the state of the fragmented ice cover. The FSD can characterize the sea-ice floe fields response to thermodynamic and dynamic atmosphere and ocean forcing. We evaluate the FSD for a series of 26 high-resolution (= 5 m) panchromatic optical satellite images that span the melt season and capture a range of sea-ice states and settings in the Canada Basin. The images are segmented for floe-area retrieval and the sensitivity to choice of parameters in the segmentation algorithm is examined. The corresponding FSDs are generally characterized by a single power law across floe scales 1,000 m to 100 km. FSDs follow a well-defined seasonal cycle of steepening into the melt season associated with the breakup of larger floes. The extensive characterization of FSDs is important for understanding the evolution of the sea-ice floe field in a changing Arctic. Results provide essential information for developing and validating theories for floe-floe interactions in the next generation of models.

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MS47

Applications of Optimal Transport in Sea Ice Dynamics

Sea ice dynamics play an important role in polar navigation and larger climate scale processes. However, there are limited observations of ice motion at navigational scales (< 1 km). It is therefore important to combine as many different information sources as possible to provide a more complete picture of the ice motion and deformation. Mathematically, this type of data fusion can be formulated as an inverse problem, where parameters in a model of the ice motion are calibrated to match satellite imagery of the ice. We will show that Wasserstein distances are a natural approach for quantitatively assessing model-data misfit in the sea ice setting and will demonstrate that recent advancements in computational optimal transport are amenable to computationally efficient gradient-based solution strategies. While our focus will be on deterministic formulations of the inverse problem, a Bayesian interpretation of the Wasserstein misfit function will also be discussed.

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MS48

Deep Learning Methods for Discovering Physics from Data

We propose unsupervised deep learning methods for deducing physical laws from data. Our work demonstrates the effectiveness of physics-constrained deep networks for dimensionality reduction and coordinate transformation as a first step for sparse identification of nonlinear dynamical systems (SINDy). First, a deep network that discovers the most physically meaningful dimensionless numbers from observations is presented. Second, we show that a deep auto-encoder can transform the coordinates of a delay-embedded time series to recover the most parsimonious dynamical system that best reconstructs it in higher dimensions. Finally, we analyze the effect of physical constraints on the robustness and extrapolation generalization of these algorithms.

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MS48

Deep Neural Network Modeling of Unknown PDEs in Nodal Space

In this talk, we present a numerical framework for deep neural network (DNN) modeling of unknown time-dependent partial differential equations (PDEs) using their trajectory data. Unlike recent work where the learning takes place in modal/Fourier space, the current method conducts the learning and modeling in physical space and uses measurement data as nodal values. We present a DNN structure that has a direct correspondence to the evolution operator of the underlying PDE, thus establishing the existence of the DNN model. The DNN model also does not require any geometric information of the data nodes. Consequently, a trained DNN defines a predictive model for the underlying unknown PDE over structureless grids. A set of examples, including linear and nonlinear scalar PDE, system of PDEs, in both one dimension and two dimensions, over structured and unstructured grids, are presented to demonstrate the effectiveness of the proposed DNN modeling. Extensions to other equations such as differential-integral equations, are also discussed.

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MS48

Physics-informed Dyna-Style Model-Based Deep Reinforcement Learning for Dynamic Control

Model-based reinforcement learning (MBRL) is believed to have much higher sample efficiency compared to traditional model-free reinforcement learning by learning a world model of the environment. However, the performance of MBRL highly relies on the quality of the learned model, which is usually built in a black-box manner and may have poor predictive accuracy outside of the data distribution. The deficiencies of the learned model may prevent the learned policy from being fully optimized. Although some uncertainty analysis-based remedies have been proposed to alleviate this issue, model-bias still poses a great challenge for MBRL, particularly when interactions with the environment are costly and limited. In this work, we propose to leverage the prior knowledge of underlying physics of the environment, where the governing laws are known or partially known. In particular, we developed a physics-informed MBRL in Dyna-style formulation, where governing equations and physical constraints are utilized to inform the model learning and policy search. By incorporating the prior information of the environment, the quality of the learned model can be notably improved, while the required interactions with the environment are significantly reduced, leading to better sample efficiency and learning performance. The effectiveness and merit have been demonstrated over a handful of classic control problems, where the environments are governed by canonical ODE/PDEs.

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MS49

High-Frequency Instabilities of Stokes Waves: A Perturbative Approach

We analyze the spectral stability of small-amplitude, periodic, traveling-wave solutions (i.e. Stokes waves) of the Euler water wave equations in finite depth. These solutions exhibit high-frequency instabilities when subject to bounded perturbations on the whole real line. We introduce a formal perturbation method to determine the asymptotic growth rates of these instabilities, among other quantities. Explicit numerical computations support our asymptotic results.

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MS49

Solitons in a Box-Shaped Wavefield with Noise: Perturbation Theory and Statistics

We investigate the fundamental problem of the nonlinear wavefield scattering data corrections in response to a perturbation of initial condition using inverse scattering transform theory. We present a complete theoretical linear perturbation framework to evaluate first-order corrections of the full set of the scattering data within the integrable one-dimensional focusing nonlinear Schrödinger (NLSE) equation. The general scattering data portrait reveals nonlinear coherent structures – solitons – playing the key role in the wavefield evolution. Applying the developed theory to a box-shaped wavefield we solve the derived equations analytically for a single Fourier mode acting as a perturbation to the initial condition, thus, leading to the sensitivity closed-form expressions for basic soliton characteristics, i.e., the amplitude, velocity, phase, and its position. With the appropriate statistical averaging, we model the soliton noise-induced effects resulting in compact relations for standard deviations of soliton parameters. Relying on a virtual soliton eigenvalue concept, we derive the probability of a soliton emergence or the opposite due to noise and illustrate these theoretical predictions with direct numerical simulations of the NLSE evolution. Finally we discuss applications of the proposed theory in description of spontaneous modulation instability development and dam-break problem. The work was supported by RSF grant No. 20-71-00022.

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MS50

Risk Structured Model of Cholera Infections in Cameroon

In this talk, we introduce a risk-structured ODE cholera model of Cameroon with no spatial structure. We use a "fitted" demographic equation (disease-free equation) to capture the total population of Cameroon, and then use a fitted low-high risk structured cholera differential equation model to study reported cholera cases in Cameroon from 1987-2004. The basic reproduction number of our fitted cholera model, R0, is bigger than 1 and our model predicted cholera endemicity in Cameroon. In addition, the fitted risk structured model predicted a decreasing trend from 1987 to 1994 and an increasing trend from 1995 to 2004 in the pre-intervention reported number of cholera cases in Cameroon from 1987 to 2004. Using the fitted risk structured cholera model, we study the impact of vaccination, treatment and improved sanitation on the number of cholera infections in Cameroon from 2004 to 2022. Furthermore, we use our fitted model to predict future cholera cases.

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MS50

Intersectionality and Climate Change Migration

As climate changes, it has both direct and indirect effects upon human migration. Sea level rise is rendering once-prime real estate uninhabitable. While billionaires build climate bunkers, low-income families find themselves priced out of their homes in the higher parts of coastal cities as the wealthy move away from their beachfront properties. Major climate events such as hurricanes and droughts are increasing in frequency and severity, causing sometimes temporary and sometimes permanent relocation. Hurricane Katrina, for example, had a disproportionately disastrous effect on Black residents of New Orleans. What insights can mathematical models give into the disproportionate effects climate change is having on various intersectional identities?

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MS50

Modeling Testing Strategies to Reduce SARS-COV-2 Transmission

As vaccines against SARS-CoV-2 are not yet available for everyone, it is important that a variety of non-pharmaceutical interventions such as quarantine, contact tracing, social distancing, and widespread mask wearing be implemented to reduce SARS-CoV-2 transmission. Testing is a necessary factor in quantifying the number of infected individuals and reducing their interaction with the population via isolation. In addition, identifying positive cases allows public health offcials to track chains of transmission via contact tracing and prevent additional infections with quarantine. To better inform testing strategies, we develop a deterministic ordinary differential equation mathematical model for given available resources in a community. Specifically, our model includes a number of characteristics which can be attributed to the variability in testing strategies, including the sensitivity of testing, availability of testing, delay in testing results, and priority of testing. Three types of test with varying sensitivity, availability, and return time are incorporated: antibody tests, RT-PCR tests, and antigen tests. Three scenarios are considered to investigate the effects of priority testing on disease transmission: test only symptomatic individuals, equally spread available tests across all testable populations for surveillance, and prioritize tests for symptomatic individuals but use the remaining testing for surveillance. Our model can determine which allocation of testing type and strategy will most significantly decrease the infectious population (peak and du- ration) given locally available testing information, e.g. available test types and number. Such results can inform interventions.

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MS51

High-Fidelity Reconstructions of the Shape and Impedance using Scattered Data

The use of an impenetrable obstacle with an impedance boundary condition was proposed to simplify the modeling of scattering of an impinging source wave off of a penetrable obstacle, knowingly the transmission scattering problem. In this paper, we propose a framework to recover both the shape and the impedance function of an obstacle from measurements of the scattered field at multiple frequencies. In our framework, we apply the recursive linearization algorithm (RLA) framing at each frequency the inverse problem as a nonlinear optimization problem. The single frequency inverse problem to recover the shape and impedance is both nonlinear and ill-posed. To deal with the nonlinearity, we apply the a Newton-like method advancing both variables, the shape and impedance function, using the Fréchet derivative of the forward operator. We treat ill-posedness by considering the approximation of the shape and impedance function to be bandlimited functions, where the limit is a function of the incident wave frequency. We present examples to demonstrate the feasibility of the method in different settings. The framework presented can recover the shape and impedance function with high accuracy when the scattered measurements used are generated by forward models with Dirichlet, Fourier-Robin or Neumann boundary conditions.

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MS51

Edge and Corner Preconditioners in Three Dimensions

In this talk, we present an RCIP-type scheme for discretizing corner and edge singularities in three dimensions. The resulting scheme attempts to discretize the geometric singularities simultaneously and solves the resulting system in a weak sense. We demonstrate the performance of the algorithm in the context of the FMM-based field solvers.

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MS51

Low Rank Compression in the Numerical Solution of the Nonequilibrium Dyson Equation

We propose a method to improve the computational and memory efficiency of numerical solvers for the nonequilibrium Dyson equation (NDE), which appears in simulations of the effect of strong radiation fields on atoms and molecules, quantum materials, nuclear physics, and many other many-body quantum systems. The NDE is a coupled system of nonlinear Volterra integral equations, for which the history integrals lead to $\mathcal{O}(N^3)$ computational complexity and $\mathcal{O}(N^2)$ memory complexity for N time steps in traditional solvers. Our method is based on the empirical observation that for many problems of physical interest, the kernels of the integral operators in the NDE, as well as its solutions, can be represented as hierarchical off-diagonal low rank (HODLR) matrices. We present an algorithm which builds these HODLR representations on the fly during the course of time stepping, and uses the them to reduce the cost of computing history integrals. For systems with the hierarchical low rank property, our method achieves $\mathcal{O}(N^2 \log N)$ computational complexity and $\mathcal{O}(N \log N)$ memory complexity. We present numerical examples demonstrating orders of magnitude speedup and memory reduction over previous methods, and reaching unprecedented propagation times.

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MS51

Efficient Numerical Methods for Initial Value Control Problems

We present fast numerical algorithms for optimal control problems with initial value control. Our contributions are the design of efficient computational methods for numerical optimization, their analysis, and their application to real-world problems. The inverse problem we are considering is commonly referred to as diffeomorphic image registration. In our formulation, we seek to find an initial momentum, which represents the initial state of a differential equation in the group of diffeomorphisms. This diffeomorphism establishes a pointwise correspondence between two images of the same object or scene, e.g., acquired at two different timepoints (the input data to our problem). We will showcase results for applications in medical imaging sciences. We will consider different formulations for this problem, and discuss the rate of convergence, accuracy, time-to-solution, and inversion quality of our formulations.

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MS52

Scientific Discovery via Spectral Analysis of Dynamical Systems

The spectral theory of dynamical system provides a powerful mathematical framework for identifying observables with a coherent (e.g., persistent or cyclical) temporal evolution through spectral decomposition of Koopman or transfer operators. From a learning perspective, such observables provide a distinguished class of features which are compatible with the dynamics, and can facilitate scientific discovery from analysis of high-dimensional time series data. In this talk, we describe how machine learning approaches, and in particular kernel methods, can be employed for spectral approximation of evolution operators on observables of dynamical systems with consistency guarantees in the large-data limit. Using idealized systems and real-world examples from climate science, we illustrate how these methods provide physically interpretable representations of coherent patterns generated by complex dynamics.

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MS52

Sparse Model Identification for Dynamical Systems with Hidden Variables

Inferring the structure and dynamical interactions of complex systems is critical to understanding and controlling their behavior. One can frame the inference problem as selecting from a library of possible terms the interactions, or model terms, most likely responsible for the observed dynamics. Despite the increased availability of data, we often do not have access to measurements of all relevant state variables, which greatly increases the challenge of model selection. Methods for the discovery of chaotic systems with hidden variables have been particularly tantalizing since in the early 80s Taken showed that the chaotic manifold structure could be constructed from time-delays of a subset of variables. Yet, until now, reconstruction of the manifold has not led to a method for model discovery in the correct coordinates. I will discuss a parameter estimation and model selection method for chaotic systems with hidden or unmeasured variables. We use a data-assimilation strategy coupled with sparsity constraints. We apply our method to experimental data from an electronic circuit well-characterized by the Lorenz system with one hidden variable. I will also discuss issues of method robustness and computational scaling

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MS52

Dynamical Systems with an Unknown Observation Function

A low-dimensional dynamical system is observed in an experiment as a high-dimensional signal, e.g., a video of a chaotic pendulums system. Assuming that we know the dynamical model up to some unknown parameters, can we estimate the underlying system's parameters by measuring its time-evolution only once? The key information for performing this estimation lies in the temporal inter-dependencies between the signal and the model. We present a kernel-based score to compare these dependencies, and then estimate the system's underlying parameters by maximizing the proposed score. We apply out method to two chaotic dynamical systems - the double pendulum and the Lorenz '63 model.

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MS53

Topological Insulators and Nonlinear Waves

Longitudinally driven periodic optical lattices, called 'Floquet Topological Insulators' and properties will be discussed. They admit a class of linear and nonlinear edge waves that propagate unidirectionally without backscatter from defects along boundary edges. The envelope of the underlying discrete nonlinear edge wave satisfies the classical integrable Nonlinear Schrödinger equation. If time permits effects due to nonlinearity will mentioned.

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MS53

Giant Vortices in Liquid Light

The existence of quantized vortices is a hallmark of superfluidity and Bose-Einstein condensates. In equilibrium condensates only quantum vortices of unit topological charge are stable, due to the dynamical instabilities of multiply charged vortices, unless supported by strong external rotation. Here we show that in Bose-Einstein condensates of exciton-polariton quasiparticles pumped in an annular geometry, not only do the constant particle fluxes intrinsic to the system naturally stabilize multiply charged vortex states, but that such states can form spontaneously through a dynamical symmetry breaking mechanism. We elucidate the properties of these novel states, notably finding that they radiate acoustically at topologically quantized frequencies. We show that the vorticity of these fluids of light are fundamentally limited by a quantum Kelvin-Helmholtz instability, and therefore by the condensate radius and pumping intensity.

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MS53

Superharmonic Instability of Stokes Waves

The classical problem of water waves on the surface of an ideal fluid in 2D is considered. We provide new insight into the stability of the Stokes waves by identifying previously inaccessible branches of instability in the equations of motion for fluid. We find that eigenvalues of the linearized problem that become unstable follow a self-similar law as they approach instability threshold, and a power law is suggested for unstable eigenvalues in the immediate vicinity of the limiting Stokes wave. The theoretical explanation of the self-similar nature of the instability branches remains an open problem.

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MS53

On Integrable Systems Gauge Equivalent to Duality Equations

After a proper gauge transformation, the self-duality reduction of Yang-Mills equation leads to an integrable system that can be studied in the spaces of different signatures. Signature (2+2) leads to a hyper-hyperbolic system with two time-like variables. Elimination of one time variable leads to the relativistic invariant system in (2+1) dimensional space that was studied in (1977). We offer a much more general class of reductions of (2+2) systems that generates new classes of integrable systems in (2+1) dimensions. Finally, we discover integrable relativistic invariant systems in full 3-dim coordinate space.

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MS54

Study Groups and Think Tanks. Hands on Industrial Training for Faculty and Post-Graduate Students

For over fifty years Study Groups have proved to be a remarkably effective mechanism for engaging mathematicians with industry, generating a strong transfer of knowledge, training, and enthusiasm for collaborative working, and of training students and faculty in the techniques needed to engage with industry. Whilst lasting under a week, they have been the route to long term engagement, training, and much new mathematics. A development of these have been Integrative Think Tanks (ITTs) in which the training aspects of engagement with industry are emphasised for PhD students. Following the COVID-19 lock down these have been transformed into Virtual Study Groups (VSGs), in which teams of mathematicians, especially students have worked on COVID-19 related problems ranging from reopening schools, HE and retail, to running trains, and conducting heart operations. The results from these in the UK have fed directly into government policy. Knowing that their work has been important in the fight against COVID-19 has been a transformative experience for the PhD students who have taken part in these events. In this talk I will describe both the mechanism of Study Groups, VSGs, ITTs, and also the creation of V-KEMS, the Virtual Forum for Knowledge Exchange in the Mathematical Sciences, which has acted to organise these events and to ensure that the work done in the VSGs gets to the right end users where it can make a real difference.

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MS54

K12 and the M3 Challenge

Engaging in the mathematical modeling process is an ideal way to prepare students for the real-world and create a workforce capable of tackling the wide range of problems ahead. In this talk, we highlight how early classroom experiences in mathematical modeling can be integrated into the curriculum and have an impact. In particular, faculty and industrial partners can play a role in helping teachers and students can confidence in math modeling. The SIAM Mathworks Math Modeling Challenge is an excellent example of this. Furthermore, most of the strategies and resources presented here can be extended to the undergraduate curriculum.

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MS55

A Functional Analysis Approach to the Static Replication of European Options

The replication of any European contingent claim by a static portfolio of calls and puts with strikes forming a continuum, formally proven by Carr and Madan (1998), is part of the more general theory of integral equations. We use spectral decomposition techniques to show that exact payoff replication may be achieved with a discrete portfolio of special options. We discuss applications for fast pricing of vanilla options that may be suitable for large option books or high frequency option trading, and for model pricing when the characteristic function of the underlying asset price is known.

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MS55

A General Framework for Optimal Investment Under Stochastic Local Volatility Models

In this paper, we propose a general framework for solving optimal investment problems (e.g. utility maximization problems) when the underlying asset follows one-dimensional or a specific type of two-dimensional Markov processes, e.g. stochastic local volatility models, which include Heston model and SABR model. It is based on a novel application of the continuous-time Markov chain (CTMC) approximation to the underlying asset price process. We manage to solve the optimal value function and the optimal strategy explicitly for the case of log utility function, and semi-explicitly for the case of power utility functions, and establish the convergence of the closed-form formula to the true value function. Extensive numerical experiments shows the accuracy and efficiency of the proposed approach.

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MS55

Dispersion-Constrained Martingale Schrdinger Problems and the Exact Joint S&P 500/VIX Smile Calibration Puzzle

Since VIX options started trading in 2006, many researchers have tried to build a model that jointly and exactly calibrates to the prices of S&P 500 (SPX) options, VIX futures and VIX options. So far the best attempts, which used parametric continuous-time jump-diffusion models on the SPX, could only produce approximate fits. In this talk we solve this longstanding puzzle using a completely different approach: a non-parametric discrete-time model. The model is cast as a dispersion-constrained martingale Schrodinger problem which is solved using the Sinkhorn algorithm. We prove by duality that the existence of such a model means that the SPX and VIX markets are jointly arbitrage-free. The algorithm identifies joint SPX/VIX arbitrages should they arise. Our numerical experiments show that our algorithm performs very well in both low and high volatility environments. Finally, we discuss how our technique extends to continuous-time stochastic volatility models, via what we dub VIX-constrained martingale Schrodinger bridges.

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MS55

Optimal Hedging under Fast-Varying Stochastic Volatility

In a market with a rough or Markovian mean-reverting stochastic volatility there is no perfect hedge. Here it is shown how various delta-type hedging strategies perform and can be evaluated in such markets. A precise characterization of the hedging cost, the replication cost caused by the volatility fluctuations, is presented in an asymptotic regime of rapid mean reversion for the volatility fluctuations. The optimal dynamic asset based hedging strategy in the considered regime is identified as the so-called 'practitioners' delta hedging scheme. It is moreover shown that the performances of the delta-type hedging schemes are essentially independent of the regularity of the volatility paths in the considered regime and that the hedging costs are related to a vega risk martingale whose magnitude is proportional to a new market risk parameter.

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MS56

On the Variation of of Bi-Periodic Waves in the Transverse Direction

Bi-periodic patterns of waves that propagate in the x direction with amplitude variation in the y direction are generated in a laboratory. The amplitude variation in the y direction is studied within the framework of the vector (vNLSE) and scalar (sNLSE) nonlinear Schrödinger equations using the uniform-amplitude, Stokes-like solution of the vNLSE and the Jacobi elliptic sine function solution of the sNLSE. The wavetrains are generated using the Stokes-like solution of vNLSE; however, a comparison of both predictions shows that while they both do a reasonably good job of predicting the observed amplitude variation in y, the comparison with the elliptic function solution of the sNLSE has significantly less error. Additionally, for agreement with the vNLSE solution, a third harmonic in y term from a Stokes-type expansion of interacting, symmetric wavetrains must be included. There is no evidence of instability growth in the x-direction, consistent with the work of Segur and colleagues, who showed that dissipation stabilizes the modulational instability. There is some extra amplitude variation in y, which is examined via a qualitative stability calculation that allows symmetry breaking in that direction.

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MS56

Conservation Laws and Multiple Scales Methods for Free-Boundary Problems in Water Waves

We consider a nonlocal formulation of the water-wave problem for a free surface with an irrotational flow, and show how the problem can be reduced to a single equation for the interface. The formulation is also extended to constant vorticity and interfacial flows of different density fluids. We show how this formulation can be used to systematically derive Olvers conservation laws not only for an irrotational fluid, but for constant vorticity and interfaces. This framework easily lends itself to computing the related conservation laws for various asymptotic models via a non-traditional approach to multiple-scales expansions.

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MS56

Ocean-Depth Measurements using Shallow-Water Wave Models

The shape of the bottom boundary of the ocean impacts a number of physical and biological processes. In this talk, within the context of shallow-water models, I will present a method to recover the bottom-profile given only measurements of the free-surface deviation. Starting from a relatively inaccurate initial guess for the bottom-boundary, reconstruction is possible for two different shallow-water models both of which are members of a class of such equations. Lastly, I will emphasize the role played by model selection in designing the reconstruction algorithm. This is joint work with Manisha and Didier Auroux.

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MS56

Quasi-Periodic Water Waves

We present a framework to compute and study two-dimensional water waves that are quasi-periodic in space and/or time. This means they can be represented as periodic functions on a higher-dimensional torus by evaluating along irrational directions. In the spatially quasi-periodic case, the nonlocal Dirichlet-Neumann operator is computed using conformal mapping methods and a quasi-periodic variant of the Hilbert transform. In the temporally quasi-periodic case, we devise a shooting method to compute standing waves with 3 quasi-periods as well as hybrid traveling-standing waves that return to a spatial translation of their initial condition at a later time. Many examples will be given to illustrate the types of behavior that can occur.

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MS57

Fresnel Diffraction for Starshade Design using the Non-Uniform FFT

Monochromatic wave scattering from planar apertures and occulters is often modeled in the scalar Fresnel diffraction approximation. The downstream (target plane) amplitude is a 2D convolution of the aperture function with a complex Gaussian $e^{i\kappa(x^2+y^2)}$. For sharp-edged scatterers the aperture function is discontinuous, rendering grid-based FFT methods at best 2nd-order accurate, leading to adoption of slower "edge-integral" methods (not to be confused with boundary integral equation methods!) I present a fast algorithm that uses high-order areal quadrature over the aperture and a single 2D nonuniform fast Fourier transform (NUFFT) to evaluate rapidly at all targets (of order 10^7 targets/second). Its cost is $\mathcal{O}(n^2 \log n)$, where n is the in-plane resolution, vs $\mathcal{O}(n^3)$ for edge-integral methods. This gives between 2 and 5 orders of magnitude acceleration when many targets are needed. Its benign scaling with Fresnel number (number of oscillations in the complex Gaussian) allows 10^3 to be reached on a laptop. I apply this to the modeling of "starshades"—30-meter diameter space-based occulters carefully shaped to shadow the direct light of a star reaching a space telescope, while allowing imaging of its planets (a billion times dimmer). Design requires many simulation runs, and 6-digit accuracy to model the deep shadow. The new code is roughly $10^4\times$ faster than the state of the art.

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MS57

An O(k Log(k)) Algorithm for the Simulation of Scattering from a Radially Symmetric Potential in Two Dimensions

Standard algorithms for solving the variable coefficient Helmholtz equation in two spatial dimensions have running times which scale at least quadratically with the wavenumber k of the problem. We will describe an algorithm with a running time which grows as k log(k), but which only applies in the special case of radially symmetric potentials.

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MS57

Fast Boundary Integral Methods for Dense Rigid Suspensions in Stokes Flow

Stokesian particle suspensions are important models of soft matter, omnipresent in nature and industry. They are crucial models to the study of biological media self-assembly and both nano and micro-structural smart materials. In this talk, we present a general computational framework for the simulation of dense Stokesian suspensions in 3D featuring boundary integral formulations for inter-particle interactions, fast evaluation schemes and optimization-based collision resolution. We present three case studies applying this framework to simulate self-assembly and complex suspension flows of spherical Janus particles (i.e. particles displaying two distinct physical or chemical properties on their surface). We will also discuss ongoing work extending our integral operator evaluation schemes to non-spherical shapes.

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MS57

Evaluating Laplace Layer Potentials Using Complex Polynomial and Plane Wave Expansions

The quadrature by expansion (QBX) technique accurately evaluates the layer potentials with singular kernels in the integral equation reformulations of partial differential equations. The idea is to form a local complex polynomial or partial wave expansion centered at a point away from the boundary to avoid the singularity in the integrand, and then extrapolate the expansion at points near or exactly on the boundary. We derive new representations of the Laplace layer potentials using both the local complex polynomial and plane wave type expansions. Unlike in the QBX, the complex polynomial expansion in the new quadrature by two expansions (QB2X) method collects the far-field contributions and its number of expansion terms can be analyzed using tools from the classical fast multipole method (FMM). The plane wave type expansion in the QB2X method is derived by first applying the Fourier extension technique to the density and polynomial approximation of the boundary geometry, and then analytically evaluating the integral using the Residue Theorem. The plane wave type expansion accurately captures the high-frequency properties of the layer potential that are determined only by the local features of the density function and boundary geometry and the nonlinear impact of the boundary on the layer potential becomes explicit. The QB2X technique allows high order numerical discretizations and can be adopted easily in existing FMM based fast integral equation solvers.

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MS58

The Neumann Problem for the Fractional Laplacian

We study a Neumann problem for the fractional Laplacian. We start with some basic properties, such as its variational formulation, probabilistic interpretation, existence of solutions, and then turn our attention to their regularity.

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MS58

Nonlocal Variational Problems: Structure-Preservation During Relaxation?

Nonlocal variational problems arise in various applications, such as in continuum mechanics through peridynamics, the theory of phase transitions, or image processing. Naturally, the presence of nonlocalities leads to new effects, and the standard methods in the calculus of variations, which tend to rely intrinsically on localization arguments, do not apply. This talk addresses the relaxation of two classes of functionals double-integrals and nonlocal supremals. Our focus lies on the question of whether the resulting relaxed functionals preserve their structure. We give an affirmative answer for nonlocal supremals in the scalar setting, along with a closed representation formula in terms of separate level convexification of a suitably diagonalized supremand, and discuss results in the vectorial case. As for double-integrals, a full understanding of the problem is still missing. We present the first counterexample showing that weak lower semicontinuous envelopes fail to be double-integrals in general. On a technical level, both findings rely on a characterization of the asymptotic behavior of (approximate) nonlocal inclusions via Young measures, a theoretical result of independent interest.

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MS58

Analysis of Self-Repulsive Curvature Energies in Relation to Harmonic Maps

I will report about progress in the theory of minimizing and critical curves and possibly surfaces under self-repulsive curvature energies. These curvature energies (among them O'Hara, Tangentpoint type energies) are nonlocal in nature, and very little is known in the scale-invariant case. This is based on joint works with S. Blatt, Ph. Reiter, and N. Vorderobermeier.

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MS58

Nonlocal Minimal Surfaces and Applications

We will present some recent developments about nonlocal minimal surfaces in terms of (ir)regularity and qualitative properties. Surfaces which minimize a nonlocal perimeter functional exhibit quite different behaviors than the ones minimizing the classical perimeter. Among these peculiar features, an interesting property, which is also in contrast with the pattern produced by the solutions of linear equations, is given by the capacity, and the strong tendency, of adhering at the boundary. In this talk, we will analyze this stickiness phenomenon from different perspectives and discuss some open problems.

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MS59

Dispersive Riemann problem for the Benjamin-Bona-Mahony equation

The Benjamin-Bona-Mahony (BBM) equation $u_t + uu_x = u_{xxt}$ as a model for unidirectional, weakly nonlinear dispersive shallow water wave propagation is asymptotically equivalent to the celebrated Korteweg-de Vries (KdV) equation while providing more satisfactory short-wave behavior in the sense that the linear dispersion relation is bounded for the BBM equation, but unbounded for the KdV equation. However, the BBM dispersion relation is nonconvex, a property that gives rise to a number of intriguing features markedly different from those found in the KdV equation. Some of these features exemplify phenomena previously observed in other dispersive equations, but some are new, providing the motivation for the study of the BBM equation as a distinct dispersive regularization of the Hopf equation. Long time dynamics of the smoothed step initial value problem or dispersive Riemann problem for BBM equation are studied using asymptotic methods and numerical simulations. Emergent wave phenomena for the dispersive Riemann problem can be roughly split into two categories: classical and nonclassical. Classical phenomena include dispersive shock waves and rarefaction waves, also observed in convex KdV-type dispersive hydrodynamics. The nonclassical features are due to nonconvex dispersion and include the generation of two-phase linear wavetrains, expansion shocks, solitary wave shedding, dispersive Lax shocks, DSW implosion and the generation of incoherent solitary wavetrains.

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MS59

Stability of Periodic Lugiato-Lefever Waves

In this talk I will describe recent advances in the stability analysis of T-periodic stationary solutions of the Lugiato-Lefever equation, a damped nonlinear Schrodinger type equation with forcing that arises in nonlinear optics. Several recent works have studied the stability of such waves to so-called "subharmonic" perturbations, i.e. NT-periodic perturbations for some natural number N. In this talk, we will instead discuss the stability of such waves to localized, i.e. integrable on the line, perturbations. As a byproduct of this analysis one can achieve subharmonic stability results which are uniform in N in both the decay rate and the domain of attraction.

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MS59

Modulation Theory for a Class of Dispersive Hydrodynamic Equations

Unidirectional dispersive hydrodynamic models typically consist of a conservation law modified by a conservative, integro-differential operator. In his 1967 paper, Whitham put forth a weakly nonlinear scalar model that matched the dispersion relation for unidirectional waves. We propose a generalization of Whitham's model consisting of a general nonlinear flux function and a general linear dispersion relation. A multiple scales calculation yields the modulation equations, a system of three conservation laws that describe the slow evolution of the periodic traveling waves wavenumber, amplitude, and mean. In the weakly nonlinear limit, explicit criteria that depend on the nonlinear flux function and linear dispersion relation are presented that establish the strict hyperbolicity and genuine nonlinearity of the modulation equations. These criteria indicate the onset of modulational instability of the finite amplitude wavetrain, and they are interpereted as a generalization of the Lighthill criterion.

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MS59

Soliton-Nonconvex Mean Flow Interaction

We present a study of soliton-mean flow interactions in the case of nonconvex systems. The loss of strict hyperbolicity is shown to be the condition for trapping of solitons within mean flows. The modified Korteweg-de-Vries equation is used as a canonical example of nonconvexity. Interaction of solitons with both classical convex mean flows and nonconvex mean flows such as kinks and contact dispersive shock waves that arise from the Riemann problem are intestigated. We show that kinks can be considered as soliton-like waves and their interaction with mean flows can also be described.

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MS61

Regularized Single and Double Layer Surface Integrals in Stokes Flow

We describe the main features of a method, developed with Svetlana Tlupova, for computing single and double layer integrals on closed surfaces in 3D Stokes flow. The integral kernel is the Stokeslet or stresslet. When evaluated near the surface, the integral is nearly singular. We obtain computed values which are uniformly about third order accurate, without needing extra resolution close to the surface. We use a quadrature rule on the surface, due to J. Wilson, which is high order accurate for smooth integrands. We discretize the integral with a regularized or smooth version of the kernel and add corrections for the error which have been derived analytically. For evaluation at points on the surface, a more special regularized kernel can be used with higher accuracy, and no correction is needed. We have verified the method with a variety of examples.

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MS61

Regularized Stokeslets: Looking Back and Moving Forward

This presentation will begin with an introduction of the method of regularized Stokeslets (MRS) for computing viscous flows generated by external forces, and the work that motivated it. The MRS was originally presented as a unified formulation that was applicable to situations where the external forces are located at scattered points, on curves, on surfaces, or in a volume. Additional regularized elements can be defined by differentiation, in analogy with the singular theory. For particular applications, the method can be specialized by selecting a regularizing function with specific properties (fast decay rate, moments, and smoothness). Examples in which forces are distributed on curves and where regularized source doublets are used will be presented. Opportunities for further extensions and possible directions for future development will be highlighted.

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MS61

Regularized Stokeslets as Means to Recover the Undisturbed Fluid Velocity in Two-way Coupled Euler-Lagrange Simulations of Particle-Laden Flows

The two-way coupled Euler-Lagrange method is widely used to simulate particle-laden flows, owing to its relatively low computational cost and the straightforward modeling of particle-particle interactions. In such simulations, the no-slip condition at the surface of each particle is not enforced, meaning that the details of the flow around the particles are not resolved on the Eulerian grid. Instead, the momentum that a particle transfers to the fluid is modeled as a single regularized momentum source, and the hydrodynamic forces acting on a particle are estimated from the underlying Eulerian flow fields, using reduced models. One major limitation of this modeling stems from the nature of the reduced models: they require access to the undisturbed flow velocity, which is the conceptual flow velocity as though the particle under consideration had been taken out of the flow domain. In this work, we propose a new idea for recovering the undisturbed flow velocity from the available disturbed Eulerian flow fields. This is done by assimilating the self-induced particle flow disturbance to a combination of regularized Stokeslets. The presence of no-slip flow domain boundaries can be accounted for by building relevant systems of images. The newly proposed framework is scrutinized by comparing its prediction of particle motion in the Eulerian-Lagrangian framework with a number of test-cases.

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MS61

Some Recent Developments in Treecodes and Ap-

plication to Regularized Stokeslets

We review a recently developed kernel-independent treecode (KITC) for fast summation of pairwise particle interactions. The method is based on barycentric Lagrange interpolation at Chebyshev points to approximate well-separated particle-cluster interactions. We present results for systems of regularized Stokeslets and rotlets in 3D, and note that the KITC is a relatively simple algorithm with low memory consumption, enabling a straightforward OpenMP parallelization. Although such treecodes can provide high accuracy approximations, the approximations are inherently discontinuous. We will also present a treecode method based on local tricubic interpolation that guarantees $\mathbb{C}^1$ continuity in the approximations.

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MS62

Optimization Based Model Order Reduction for Stochastic Systems

In this talk, we will link worlds of model order reduction for stochastic linear systems and $\mathcal{H}_2$-optimal model order reduction for deterministic systems. In particular, we supplement and complete the theory of error bounds for model order reduction of stochastic differential equations. With these error bounds, we establish a link between the output error for stochastic systems (with additive and multiplicative noise) and modified versions of the $\mathcal{H}_2$-norm for both linear and bilinear deterministic systems. When deriving the respective optimality conditions for minimizing the error bounds, we see that model order reduction techniques related to iterative rational Krylov algorithms (IRKA) are very natural and effective methods for reducing the dimension of large-scale stochastic systems with additive and/or multiplicative noise. We apply modified versions of (linear and bilinear) IRKA to stochastic linear systems and show their efficiency in numerical experiments.

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MS62

Context-Aware Model Reduction for Uncertainty Quantification

Multifidelity methods leverage low-cost surrogate models to speed up computations and make occasional recourse to expensive high-fidelity models to establish accuracy guarantees. Because surrogate and high-fidelity models are used together, poor approximations by the surrogate models can be compensated with frequent recourse to high-fidelity models. Thus, there is a trade-off between investing computational resources in training and improving surrogate models and the frequency of making recourse to high-fidelity models; however, this trade-off is ignored by traditional model reduction and data-driven modeling methods that learn surrogate models that are meant to replace high-fidelity models rather than being used together with high-fidelity models. This presentation introduces the concept of context-aware learning that aims to derive models that are explicitly trained to be used together with high-fidelity models in multi-fidelity settings. Our analysis shows that in certain situations this trade-off can be exploited explicitly, which leads to an optimal training of surrogate models. The result is that fewer data points are provably sufficient when learning models for multi-fidelity computations than when learning models to be used in single-fidelity settings.

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MS62

Multifidelity Ensemble Kalman Filtering using Physics-informed Autoencoders

The multifidelity ensemble Kalman filter aims to combine a full-order model and a hierarchy of reduced order surrogate model in an optimal statistical framework for Bayesian inference in sequential data assimilation. In this work we extend the multifidelity ensemble Kalman filter to work with non-linear couplings between the models. Using autoencoders it is possible to train optimal projection and interpolation operators, and to obtain reduced order surrogate models with less error than conventional linear methods. We show on the canonical Lorenz '96 model that such a surrogate does indeed perform better in the context of multifidelity filtering.

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MS62

Certified Reduced Order Methods for Variational Data Assimilation: A Space-Time Approach

In the process of reproducing the state dynamics of a physical system, data from physical measurements can be incorporated into a mathematical model to improve the state prediction. This process, referred to as Data Assimilation, must deal with the discrepancies between data and model arising both from the measurement noise and model inaccuracies and uncertainties. Among different methods developed, in our study, we focused on the strong 4D-VAR method. It perturbs the initial conditions in order to find a state dynamics that better justifies the physical observations, while preserving the physics of the system as described by the model. In this context, our research introduced two main novelties: for physical problems described by linear parabolic PDEs, we derived a rigorous space-time formulation of the 4D-VAR method, employing a P1-P0 Petrov-Galerkin discretization in time and reduced basis (RB) in space. In addition, we modelled the sensors as linear functional over this Bochner space. We derived efficient and effective a-posterior error bounds both for the primal and adjoin problem and for the error in the estimation of the initial condition. Besides this, we proposed an algorithm for the selection of sensors locations in space and measurement intervals in time with the goal of achieving a nearly optimal space-time experimental design. Numerical tests have been performed studying the 2D convection-diffusion of contaminants with unknown initial concentrations.

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MS63

Rational Neural Networks

The choice of the nonlinear activation function in deep learning architectures is crucial and heavily impacts the performance of a neural network. In this talk, we consider neural networks with rational activation functions. We then establish optimal bounds in terms of network complexity and prove that rational neural networks approximate smooth functions more efficiently than ReLU networks with exponentially smaller depth. The flexibility and smoothness of rational activation functions make them an attractive alternative to ReLU.

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MS63

Nonlinear Approximation and (deep) Relu Networks

This talk is concerned with the approximation power of deep neural networks, an active research area currently producing many interesting papers. The most common results found in the literature prove that neural networks approximate functions with classical smoothness to the same accuracy as classical methods, e.g. approximation by polynomials or piecewise polynomials on prescribed partitions. However, approximation by neural networks depending on n parameters is a form of nonlinear approximation and as such should exhibit the increased efficiency of nonlinear approximation methods. The present work shows that this is indeed the case. Furthermore, the performance of neural networks in targeted applications indicate that they actually possess even greater approximation power than traditional methods of nonlinear approximation, such as free knot splines or n-term approximation from a dictionary. The present work again shows that this is indeed the case. To do so, we exhibit large classes of functions which can be efficiently captured by neural networks where classical nonlinear methods fall short of the task. We purposefully limits ourselves to studying the approximation of univariate functions by ReLU networks. Many generalizations to functions of several variables and other activation functions exist. However, even in this simplest of settings, a theory that completely quantifies the approximation power of neural networks is still lacking.

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MS63

Universal Approximation for Neural Differential Equations

Differential equations and neural networks are two of the most widespread modelling paradigms. *Neural differential equations* are an emerging blend combining old and new, with applications to deep learning and the promise to revolutionise traditional mathematical modelling. I will begin with a brief introduction to the topic, its intuition, applications etc., before discussing the central theme of whether such models can be universal approximators (UAs). We shall see several key results: first that ‘unaugmented’ neural ODEs are not UAs; next that ‘augmented’ neural ODEs can be UAs whether or not their vector fields are themselves UAs; finally how neural *controlled* differential equations–featuring a time-varying input, to be thought of as ‘continuous RNNs’ – can be shown to be UAs with respect to the time-varying input path, through application of rough path theory.

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MS64

Mixed Precision Algorithms for Pushing the Performance Limits of Modern HPC Architectures

On the road to exascale computing, the gap between the compute power available in the arithmetic cores on the one hand and the bandwidth to main memory or between nodes on the other hand keeps increasing dramatically, making data access and communication prohibitively expensive compared to arithmetic operations. With no disruptive hardware changes on the horizon, we are facing a situation where all high performance computing applications suffer from the slow communication to main memory or in-between nodes. A promising strategy to overcome this problem is to utilize the bandwidth capacity more carefully, reduce the communication volume and the number of communication points, and - whenever possible - trade communication against computations. The idea is to radically decouple the memory precision from the arithmetic precision, employ high precision only in the computations, and lower the precision as much as possible when accessing data in main memory or communicating with remote processors. In this talk, we motivate and present the idea of decoupling the memory precision from the arithmetic precision, and discuss the potential and limitations of the approach in the sense of preserving the algorithm correctness. We also provide examples for bandwidth-bound numerical linear algebra algorithms that are amenable to the format separation, and evaluate the performance gains we can achieve for real-world problems on recent HPC architectures.

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MS64

Heffte: Fft Computations Towards Exascale

The fast Fourier transform (FFT), widely used by applications from various fields of science and engineering, is known to be a communication-bound algorithm, and its parallel implementation on the upcoming exascale systems need to be carefully tailored to architectural capabilities. In this talk, we present novel techniques to accelerate 2D and 3D FFT computation on hybrid CPU-GPU systems. We propose novel architecture-aware tuning techniques and present further developments on heFFTe library. We provide substantial experiments on scalability and comparison among different state-of-the-art FFT libraries. We used up to 24,576 IBM Power9 cores and 6,144 NVIDIA V-100 GPUs on Summit supercomputer, and up to 1.3 million A64fx Fujitsu cores on Fugaku supercomputer.

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MS64

When Floating-Point Error Matters: the Hazards and Challenges of Low-Precision Computation

Within the next few years, exascale-level machines will become a reality. Making use of this available computing power in applications will require a massive effort towards optimizing parallel large-scale computations. This challenge is complicated by the increasing heterogeneity of machines at the node level. Notably is the emergence of low and mixed precision hardware, the use of which offers potentially huge performance gains. A common technique in scientific computing is to introduce inexactness into the computation to reduce computation time, e.g. in model order reduction, sparsification, low-rank approximation, and randomized and communication-avoiding algorithms. In many cases, roundoff error is assumed to be orders of magnitude smaller than any approximation error, and thus the interaction between these different errors is often ignored. In the world of low precision computation, however, this may no longer be a valid assumption. We therefore ask the question: When does floating-point error matter, and what can go wrong if we use low precision blindly? This talk will give examples, summarize some existing work in this area, and explain the remaining gaps in our knowledge.

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MS64

Randomization for Solving Large Systems of Linear Equations

This talk focuses on recent advances on using randomization techniques for solving linear systems of equations. We first focus on computing sketches efficiently in parallel by using subsampled randomized hadamard transforms. Then we present a randomized Gram-Schmidt algorithm for orthogonalizing a set of vectors that has numerical accuracy close to Modified Gram-Schmidt while having the cost of classical Gram-Schmidt. We present then its usage in GMRES for solving large systems of linear equations.

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MS65

Computational Barriers in Continuous Optimization for Machine Learning

Researchers in the field of continuous optimization have repeatedly expanded and re-defined the realm of tractable optimization problems. This endeavor has culminated in the well-known class of convex optimization problems with applications in a wide range of scientific fields. In this talk, I will present the traditional oracle-based complexity model, which has dominated (unstructured) continuous optimization for the past 40 years, and highlight some of its successes and failures in predicting the hardness of convex optimization problems. I will then introduce a novel structural-based model aimed at addressing major oracle-based complexity gaps. The new approach is intimately tied with approximation theory, and is proven to be particularly advantageous for characterizing the complexity of optimization methods in machine learning.

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MS65

Lessons from Trace Estimation Lower Bounds: Testing, Communication, and Anti-Concentration

In Implicit-Matrix Trace Estimation, we are given access to a Matrix-Vector Oracle and want to estimate the trace of the underlying matrix with as few queries as possible. This classical problem has many downstream applications, from estimating log-determinants to approximate the number of triangles in a graph. This talk will briefly cover two algorithms for trace estimation. Using the intuitions underlying these algorithms, we will design and compare three lower bounds for trace estimation. All three lower bounds agree that the existing algorithms are optimal, but they rely on very different mathematical tools, and therefore give subtly different results. The majority of this talk will examine these differences: Which proofs generalize easily to other problems? How do these proofs reflect our intuitions? Do these proofs allow for additional computational constraints (e.g. non-adaptive algorithms)?

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MS65

Conditional Lower Bounds for Spectral Sums

We study the complexity of estimating *spectral sums* of the form $\sum_{i=1}^{n} f(\sigma_i(A))$ where A is an $n \times n$ matrix, $\sigma_i(A)$ is its i^{th} singular value, and $f : \mathbb{R} \to \mathbb{R}$ is some function. Examples include the matrix Schatten p-norms (including the nuclear norm), the SVD entropy, the trace inverse, the log-determinant, and many more. In recent work, we show that, using stochastic linear system solvers, many sums can be estimated to $(1+\epsilon)$ relative error in $n^{\gamma} \cdot poly(1/\epsilon)$ time, where γ is smaller than the current fast matrix multiplication constant $\omega \approx 2.37$. E.g., the nuclear norm can be approximated in $\tilde{O}(n^{2.18}/\epsilon^3)$ time. Complementing this, we show that the complexity of spectral sum approximation is inherently tied to fast matrix multiplication in the small ϵ regime. We give conditional lower bounds, showing that achieving milder ϵ dependencies in our algorithms would imply triangle detection algorithms running in faster than matrix multiplication time. This further implies that highly accurate spectral sum algorithms running in subcubic time can be used to give subcubic time matrix multiplication. As an application of our bounds, we show that precisely computing all effective resistances in a graph in less than matrix multiplication time is likely difficult, barring a major algorithmic breakthrough.

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MS65

Hardness via the Matrix-Vector Query Framework and via Reductions

Although unconditional computational hardness for problems is difficult to show, we give an overview of several methods for proving lower bounds for linear algebraic tasks. One method is to consider the matrix-vector query product setting: in this setting the algorithm is assumed to proceed by making a sequence of possibly adaptive matrix-vector products to an input matrix A, where the queries form a sequence $v_1, \ldots, v_r$ of vectors, the responses are $Av_1, \ldots, Av_r$, and the v_i can be chosen adaptively based on previous responses. We give an overview of several fundamental problems for which nearly optimal lower bounds have been shown in this setting. Another method for showing hardness is via reduction, showing that if one can solve certain linear algebraic tasks then one can solve some other problem in time faster than what is currently known, such as counting triangles in a graph or multiplying arbitrary matrices with a certain sparsity. We survey several fundamental problems for which this technique has been successful as well.

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MS66

A Periodic Fast Multipole Method

Many physical models prescribe periodic or quasiperiodic boundary conditions on a unit cell. For interacting charged particles, these boundary conditions can be imposed directly by calculating the potential induced by an infinite tiling of "images" of the charges in the unit cell. In this talk, we present a novel planewave-based representation for the potential induced by these image charges and we describe how to effectively couple this representation with a fast multipole method (FMM). The resulting scheme is effective for general parallelogram unit cells and has been implemented for several common interaction kernels.

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Accurate Integral Equation Methods Using the Layered Media Green's Function

This talk will present numerical issues evaluating the layered media Green's function for the Helmholtz equations. One of the well-known issues is the slow convergence of Sommerfeld integral when the source and target points are near the layer interface. We overcome the issue by using alternative direction formulas based on contour integrals that are equivalent to the original integrals. The alternative direction formulas converge exponentially when the Gauss-Laguerre quadrature is used. Boundary integral equations for acoustic wave scattering from objects located close to the layer interface are set up using the layered media Green's function and solved using the Nystrom method with high precision.

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MS66

Fmm-Accelerated Adjoint Methods

PDE-constrained optimization has led to many efficient techniques for the design of electrical and mechanical devices, relying on the solution of many PDEs inside an outer optimization loop. Computationally, most of these optimization procedures rely on PDE-based solvers (finite elements, etc.) of the underlying equations and adjoint methods, despite the superiority of computational integral equation methods in various regimes. In this talk well give an overview of integral equation-based FMM-accelerated methods for performing optimization using adjoint operators.

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MS66

Fmm3dbie - a High Order Solver for Boundary Value Problems in Complex 3d Geometries

Fmm3dbie (https://fmm3dbie.readthedocs.io/en/latest/) is a set of libraries to solve constant coefficient elliptic boundary value problems on surfaces in three dimensions. The library currently supports Dirichlet, Neumann, and transmission boundary value problems for Laplace, Helmholtz, and Yukawa equations; velocity, mobility and traction boundary value problems for Stokes equations; and PEC and dielectric boundary value problems for Maxwell's equations on multi-core shared memory machines. The library provides support for evaluating layer potentials on and off the surface using locally corrected precomputed quadratures, FMM accelerated iterative solvers, interfaces for matrix entry generation for dense and fast direct solvers. The solvers are capable of obtaining high order accuracy, are robust in the presence of close-to-touching features in the geometry and can interface with standard mesh formats like gmsh and TRI file format. In this talk, we will present the different locally corrected quadrature schemes used in fmm3dbie and demonstrate its capability with several numerical examples.

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MS67

Experimental Design and Identifiability in Models of Blood Coagulation

Blood coagulation is a complex network of biochemical reactions necessary for blood clots to form. To combat or enhance clotting, components of the coagulation system can be targeted by therapeutic agents, the kinetic properties of which are studied using indirect measurements of enzymatic activity and inhibition via synthetic substrates in biochemical assays. Mathematical models are thus indispensable tools that allow for interpretation of such data, elucidation of biochemical mechanisms, and experimental design. In particular, systems of nonlinear ODEs give interpretable rate equations and allow for data fitting. We recently used Bayesian parameter estimation to determine that product inhibition plays an important role in even the simplest of biochemical assays that use synthetic substrates. In this work, as a first step toward modeling more complex reactions, we consider multiple enzymes and inhibitors in the assays, for which the kinetic parameters, initial concentrations, and kinetic schemes are uncertain. It is well known that parameters in these systems can be difficult to estimate or possibly not even identifiable. The challenge is to formulate an accurate biochemical model and identify the specific experimental designs that will result in useful estimates of the process parameters. Some promising results have been obtained using Monte Carlo simulations of synthetic observations and then examining profile likelihoods to determine the identifiability of parameters.

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MS67

Quantifying Uncertainty in Time-Varying Parameters for Biological Systems

Estimating and quantifying uncertainty in system parameters remains a big challenge in many biological and biomedical applications. In particular, many such systems involve parameters that are known to vary with time but have unknown dynamics and cannot be measured. This talk will address aspects of uncertainty in ensemble-based filtering estimates of time-varying parameters, with particular emphasis on how uncertainty in the parameter estimates affects the corresponding model output predictions. Results will be demonstrated on examples from biological and biomedical systems.

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MS67

Equation Learning and Uncertainty Quantification for Biological Transport Models of Glioblastoma Growth

A recent area of research is applying machine learning methods towards learning mathematical models from data. These methods have shown promise in physical applications in which data quality and quantity is high, however, testing and extending equation learning methodology to biological settings with high noise levels and few data points has been less well investigated. We adapted and tested equation learning methods in a biologically realistic setting using the Fisher-KPP model, a commonly utilized model for describing spatiotemporal glioblastoma tumor growth and invasion. We simulated glioblastoma patient data with 1%, 5%, and 10% noise levels, generating only a few time points (either 3, 5, or 10) which could be used for equation learning. We used bootstrapping to assess parameter uncertainty in the learned equations. We found that the ability of equation learning methods to recover the correct equation and parameters was sensitive to the parameter domain, i.e., the proliferation and diffusion rates describing the tumor growth. We found that the correct equations and parameters for slower growing tumors could be recovered with as few as 3 time points.

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MS67

Sensitivity Analysis Applied to a Hemodynamic Model of the Eye

Optic neuropathies such as glaucoma are often late-onset, progressive and incurable diseases. Despite the recent progress in clinical research, there are still numerous open questions regarding the etiology of these disorders and their pathophysiology. The recent use of mathematical models applied to biomedical problems has helped unveiling complex mechanisms of human physiology. We have designed a mathematical and computational model, namely the Ocular Mathematical Virtual Simulator, in order to simulate the hemodynamics and biomechanics of the main tissue of the eye. To understand the propagation of uncertainties from input and output and to quantify the effect of parameter variability on the results, we have performed a variance-based sensitivity analysis on the hemodynamic components of our model. In particular, I will present the effect of intraocular pressure and systemic blood pressure on the ocular posterior tissue vasculature. The combination of a physically-based model with experiments-based stochastic input allows us to gain a better understanding of the physiological system, accounting both for the driving mechanisms and the data variability. Additionally, the results obtained with this analysis support the validity of the model and its clinical application.

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MS68

Manifold Embeddings with Physical Meaning

Scientific research involves finding patterns in data, formulating hypotheses, and validating them with new observations. Machine learning is many times faster than humans at finding patterns, yet the task of validating these ”discoveries” is still left to the human expert or to further experiment. My Unsupervised Validation for Unsupervised Learning program aims to design broad-ranging, mathematically and statistically grounded methods to interpret, verify and validate the output of Unsupervised Learning algorithms. Manifold embedding algorithms aim to find intrinsic coordinates that describe a data manifold, yet they return ”abstract” coordinates; domain experts must relate these with phyiscally meaningful variables, mainly by visualization or other ad-hoc procedures. We introduce a method to automate this work. Namely, to explain embedding coordinates as non-linear compositions of functions from an expert-defined dictionary. We show that this problem can be set up as a sparse linear recovery problem, find sufficient recovery conditions, and demonstrate its effectiveness on data. With this class of new methods, called ManifoldLasso, a scientist can specify a (large) set of functions of interest, and obtain from them intrinsic coordinates for her data in a semi-automatic, principled fashion.

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MS68

Dense Single-Molecule Localization Microscopy

Using Deep Learning

In biological imaging, fast acquisition of depth information is crucial e.g. for accurate 3D tracking of sub-cellular elements and for 3D super-resolution. Snapshot depth sensing is commonly achieved via wavefront coding. In this technique, the optics is modified such that the point-spread function (PSF) varies distinctively as a function of the depth of the imaged object. However, to date, this approach has shown limited success in samples with very dense emitters, due to the lateral overlaps of the emitter PSFs in the captured image. Here, we present an approach for jointly designing the PSF and the 3D reconstruction algorithm, by using deep learning. Specifically, we introduce a neural network whose training determines both a phase-mask to insert at the optical path of a micropscope, and a neural model that recovers 3D positions of point emitters from their imaged PSFs. We demonstrate our approach experimentally with super-resolution reconstructions of mitochondria and volumetric imaging of fluorescently labeled telomeres in cells. Our method, DeepSTORM3D, enables the study of biological processes in whole cells at timescales that are rarely explored in localization microscopy. We also present a multi-channel variant of DeepSTORM3D, in which the optical signal is split to two sensors. Here, end-to-end learning of two phase masks allows us to double the detection rate and to reach improved precision compared to the single-channel design.

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MS68

Operator Inference for Learning Reduced Models with Non-Markovian Terms from Partially Observed State Trajectories

This work introduces a non-intrusive model reduction approach for learning reduced models from partially observed state trajectories of high-dimensional dynamical systems. The proposed approach compensates for the loss of information due to the partially observed states by constructing non-Markovian reduced models that make future-state predictions based on a history of reduced states, in contrast to traditional Markovian reduced models that rely on the current reduced state alone to predict the next state. The core contributions of this work are a data sampling scheme to sample partially observed states from high-dimensional dynamical systems and a formulation of a regression problem to fit the non-Markovian reduced terms to the sampled states. Under certain conditions, the proposed approach recovers from data the very same non-Markovian terms that one obtains with intrusive methods that require the governing equations and discrete operators of the high-dimensional dynamical system. Numerical results demonstrate that the proposed approach leads to non-Markovian reduced models that are predictive far beyond the training regime. Additionally, in the numerical experiments, the proposed approach learns non-Markovian reduced models from trajectories with only 20% observed state components that are about as accurate as traditional Markovian reduced models fitted to trajectories with 99% observed components.

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MS69

Phase Field Method for Mass Transfer Through Permeable Bio-Membranes

In this work, we develop a new mathematical model for mass transfer phenomenon with the help of phase field method. The resulting model is a coupled system including Navier-Stokes equations, Cahn-Hilliard equation and a reaction-diffusion equation with variable diffusion coefficient. The sharp interface limit is also conducted. Besides, we establish a decoupled, linear and unconditional energy stable numerical scheme to solve this system efficiently. The centered-block finite difference method with stagger mesh is made use of discretization in space. Some numerical experiments are carried to varify our theoretical result and explain this new model.

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MS69

Variational Schemes to Generalized Diffusions, Gradient Flows and Beyond: A Discrete Energetic Variational Approach

In this talk, we present a systematic framework of deriving variational numerical schemes for generalized diffusions and gradient flows. The proposed numerical framework is based on the energy-dissipation law, which describes all the physics and the assumptions in a given system and can combine different types of spatial discretizations including both Eulerian and Lagrangian approaches. The resulting semi-discrete equation inherits the variational structures from the continuous energy-dissipation law. As examples, we apply such an approach to construct variational Lagrangian schemes to porous medium type generalized diffusions and Allen-Cahn type phase-field models, and particle methods for variational inference. Numerical examples show the advantages of variational Lagrangian schemes in capturing singularities, thin diffuse interfaces, and free boundaries.

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MS69

A Tridomain Model for Optic Nerve Microcirculation

Flows of water and various organic and inorganic molecules in the central nervous system are important in a wide range of biological and medical processes, as has recently become apparent (Nedergaard and Goldman 2020). However, the exact mechanisms that drive these flows are often not known. Here we investigate the forces and flows in a tridomain model of the central nervous system. We use the experimental system of the optic nerve, investigated by the Harvard group (Orkand, Nicholls, and Kuffler 1966) as a protype of the central nervous system in general. We construct a model and choose its parameters to fit the experimental data in detail. Our model is three dimensional and is meant to include significant anatomical detail in a general way. In this way, the model can be adapted to describe other systems with other structures, channels and transporters.

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MS70

New Results for Collisionless Damping in Relativistic Plasmas

In this talk I discuss new theoretical and computational results for relativistic Landau damping. The plasma dispersion function is solved to machine precision using direct line integration in the complex plane, in combination with an analytic evaluation of the residue to account for the deformation along the Landau contour. The approach is generic in that it applies to arbitrary distribution functions, and numerical subtleties related to the placement of the contour are discussed. As is well-known, we confirm that the Landau root becomes increasingly undamped as the plasma becomes hotter, and furthermore show that the Landau root ceases to exist for sufficiently relativistic plasmas. Connection to full phase-space Vlasov simulation is provided by discussing results from the 2D+2P Vlasov code LOKI. Building on prior work, we address the significant computational cost associated with high-dimensional phase space approximation using high-order accurate numerical schemes as a means to reduce the cost required to deliver a given level of error in the computed solution. Fully conservative and minimally diffuse difference formulations of order four and six are used.

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MS70

Effective Dispersion Relations and Linearization of Nonlinear Waves

Effective dispersion arises in a number of weakly nonlinear wave systems, typically from the leading-order nonlinear self-interactions of waves, and implies that nonlinear waves act approximately, on average, like collections of linear dispersive waves. This talk describes how nonlinear dispersion also arises for moderately and even highly nonlinear waves in systems such as the Majda-McLaughlin-Tabak model of wave turbulence, the Fermi-Pasta-Ulam chain, and the Nonlinear Schroedinger Equation. For the first two, we describe how effective dispersion arises even in the case in which linear dispersion is absent. For the Nonlinear Schroedinger Equation, we show that, counterintuitively, the approximation by the Effective Dispersion Relation improves with wave amplitude, and yields an effective linearization of waves in the infinite-amplitude limit. This work was initiated by the late David Cai.

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MS70

Magnetic Filamentation in the Convective Zone of the Sun

We discuss the question about magnetic collapse as a possible process for the singularity formation of the magnetic field for a finite time in the framework of the ideal incompressible MHD. This process is important for the formation of magnetic filaments in the convective zone of the Sun. The possibility of the collapse is connected with the compressibility of the magnetic field lines (E.A. Kuznetsov, T. Passot, P.L. Sulem, Phys. Plasmas 11, 1410 (2004)). One of the well-known examples of the formation of magnetic filaments with known velocity field first considered by Parker in 1963 (E.N. Parker, Astrophysical Jour. 138, 552 (1963)) demonstrates rather that the magnetic field growth has exponential character. It is shown that due to the frozenness of the magnetic field within the kinematic approximation for the induction equation the formation of filaments with the exponential growth of the magnetic field takes place on regions with hyperbolic velocity profile (E.A. Kuznetsov, E.A. Mikhailov, JETP 131, 496505 (2020)). Due to account of the magnetic viscosity which destroys the magnetic field frozenness, this growth saturates at the level $B_0 Re_m^{-1/2}$ where B_0 is the initial magnetic field strength and Re_m is the magnetic Reynolds number. For the Solar convective zone, this value reaches 1 KG or even more. This work was performed under the financial support of the Russian Science Foundation (grant no. 19-72-30028).

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MS70

Generalized Constantin-Lax-Majda Equation: Collapse vs. Blow Up and Global Existence

We investigate the behavior of the generalized Constantin-Lax-Majda (CLM) equation which is a 1D model for the advection and stretching of vorticity in a 3D incompressible Euler fluid. Similar to Euler equations the vortex stretching term is quadratic in vorticity, and therefore is destabilizing and has the potential to generate singular behavior, while the advection term does not cause any growth of vorticity and provides a stabilizing effect. We study the influence of a parameter a which controls the strength of advection, distinguishing a finite time singularity formation (collapse or blow-up) vs. global existence of solutions. We find a new critical value $a_c = 0.6890665337007457...$ below which there is finite time singularity formation that has a form of self-similar collapse, with the spatial extent of blow-up shrinking to zero, and above which up to $a = 1$ we have an expanding blow up solutions. We identify the leading order complex singularity for general values of a which controls the leading order behavior of the collapsing solution. We also rederive known exact analytical collapsing solutions for $a = 0$ and $a = 1/2$ using this approach. For $a_c < a \leq 1$, we find a blow-up solution on the real line in which the spatial extent of the blow-up region expands infinitely fast at the singularity time. For $a > 1$, we find that the solution exists globally with exponential-like growth of the solution amplitude in time. Reference: arXiv:2010.01201

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MS71

Title: Data Driven Learning of Robust Nonlocal Models: from Molecular Dynamics to Nonlocal Models for Continuum Mechanics

In this talk I will present an operator-regression technique to obtain accurate surrogates that reproduce molecular dynamics (MD) simulations at coarser scales. Starting from MD data of graphene at different temperatures, we first apply a coarse-graining technique to project the data onto a much coarser grid and then use coarse-grained data to train a nonlocal model that accurately reproduces MD data from a validation set. Our results for a perfect crystal and in presence of thermal noise illustrate the excellent generalization properties of our learning algorithm.

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MS71

Approximation of Integral Fractional Laplacian and Fractional PDEs via Sinc-Basis

We introduce a spectral method to approximate the fractional Laplacian employing a sinc basis. Using our scheme, the evaluation of the operator and its application onto a vector has complexity of $\mathcal{O}(N \log(N))$ where N is the number of unknowns. Thus, using iterative methods such as conjugate gradient, we provide an efficient strategy to solve fractional partial differential equations with homogeneous exterior Dirichlet conditions on arbitrary Lipschitz domains. Our implementation works in arbitrary dimension and we further illustrate its efficiency by applying it to fractional Allen-Cahn and image denoising problems. Finally we discuss issues of convergence analysis for this method, noting that experimentally we recover the same convergence rates for certain benchmark problems as predicted by numerical analysis of finite-element-based methods.

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MS71

Optimal Control of Fractional PDEs

In the first part of this talk, we discuss a novel Deep Neural Network (DNN) which allows connectivity between all the layers. The latter is accomplished by using of fractional time derivatives. We apply the resulting fractional-DNN to learn parameter to solution map in parameterized partial differential equations (PDEs). Subsequently, we use this approximation to solve Bayesian inverse problems. We observe a speedup of 100x over the existing approaches. In the second part of this talk, we shall focus on yet another nonlocal/fractional operator, i.e., fractional Laplacian. By appealing to the nonlocal nature of this operator, we introduce a completely novel class of inverse/optimal control problems. We conclude the talk by studying the regularity and designing Moreau-Yosida regularization based optimization algorithms for state constrained optimal control problems with fractional PDEs as constraints.

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MS72

The Unified Transform Method for Linear Semi-

Discrete Evolution IBVPs

In this work, we present a semi-discrete analogue of the Unified Transform Method proposed by A. S. Fokas to solve initial-boundary value problems for evolution linear partial differential equations. The semi-discrete method is presented via applications to spacial discretizations of several linear equations on the half-line $x \geq 0$ and on the finite interval $x \in [0, L]$. We discuss the continuum limit of the integral solutions and numerical results.

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MS72
Analytic Continuation of Solutions of Initial-Boundary Value Problems Outside the Domains

The Unified Transform Method (UTM), or the method of Fokas, gives solutions to half-line and finite-interval, linear, constant-coefficient initial and boundary value problems (IBVPs) as contour integrals over a spectral parameter with the space and time variables as parameters in the integral. The contour integrals are defined when the space variable is inside the domain of the problem. We extend the space variable outside the domain and find the appropriate initial conditions that would generate the same solution inside the domain. In general, the extended initial condition is not differentiable or continuous unless the boundary and initial conditions satisfy some compatibility conditions. We analyze both dispersive and dissipative IBVPs.

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MS72
The Phenomenon of Dispersive Revivals

I will give an introduction and discuss recent results to the phenomenon of "dispersive quantization" or "revivals". Although first reported in 1835 by Talbot, this phenomenon was only studied in the 90s, in particular for the periodic free space Schrodinger equation by Berry and al. It was then rediscovered for the Airy equation by Peter Olver in 2010. Since then, a sizeable literature has examined revivals for the periodic problem for linear dispersive equations with polynomial dispersion relation. What I will discuss in this talk is further occurrences of this phenomenon for different boundary conditions, a novel form of revivals for more general dispersion relations and nonlocal equations such as the linearized Benjamin-Ono equation, and nonlinear (integrable) generalizations. This work is joint with Lyonell Boulton, George Farmakis, Peter Olver and David Smith.

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MS72
Linear Evolution Equations on the Half Line with Dynamic Boundary Conditions

The classical half line Robin problem for the heat equation may be solved via a spatial Fourier transform method. In this talk, we study the problem in which the static Robin condition $bq(0,t) + qx(0,t) = 0$ is replaced with a dynamic Robin condition; $b = b(t)$ is allowed to vary in time. We present a solution representation, and justify its validity, via an extension of the Fokas transform method. We show how to reduce the problem to a variable coefficient fractional linear ordinary differential equation for the Dirichlet boundary value. We implement the fractional Frobenius method to solve this equation, and justify that the error in the approximate solution of the original problem converges appropriately. We also demonstrate an argument for existence and unicity of solutions to the original dynamic Robin problem for the heat equation. Finally, we extend these results to linear evolution equations of arbitrary spatial order on the half line, with arbitrary linear dynamic boundary conditions.

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MS73
Applications of the Singular Value Decomposition in Media Processing and Watermarking Schemes

The singular value decomposition, or the SVD, was first discovered independently by Eugenio Beltrami and Camille Jordan in the 1870s as they were tackling problems related to bilinear forms in linear algebra. Since then, it has become one of the most useful tools in linear algebra, seeing applications in widely disparate fields. In our presentation, we introduce applications of the SVD in image processing, audio processing, and digital ownership protection. We provide several examples illustrating applications and properties of the SVD, including image compression, image and audio processing, video background extraction, and watermarking for digital ownership protection. Finally, we propose a modified version of a watermarking scheme introduced in Jain, Arora, and Panigrahi, A reliable SVD based watermarking scheme, CoRR abs/0808.0309 (2008) which offers improved robustness and imperceptibility properties. Faculty Advisors: Minah Oh, James Madison University, ohmx@jmu.edu

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MS73
Origami Hexagon Deformations and Flip Graph

By utilizing origami folding processes, researchers have been able to solve a wide range of engineering problems such as fabricating different robot morphologies and manufacturing folding-based mechanisms. Leveraging origami structures with given crease pattern requires geometric and numerical understanding of folding configurations. Faculty Advisors: Richman, Harry, University of Washington, hrichman@uw.edu

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MS73

Factor-$\sqrt{2}$ Acceleration of Accelerated Gradient Methods

The optimized gradient method (OGM) provides a factor-$\sqrt{2}$ speedup upon Nesterov's celebrated accelerated gradient method in the convex (but non-strongly convex) setup. However, this improved acceleration mechanism has not been well understood; prior analyses of OGM relied on a computer-assisted proof methodology, so the proofs were opaque for humans despite being verifiable and correct. In this work, we present a new analysis of OGM based on a Lyapunov function and linear coupling. These analyses are developed and presented without the assistance of computers and are understandable by humans. Furthermore, we generalize OGM's acceleration mechanism and obtain a factor-$\sqrt{2}$ speedup in other setups: acceleration with a simpler rational stepsize, the strongly convex setup, and the mirror descent setup. Faculty Advisors: Ernest, Ryu, Department of Mathematical Sciences, Seoul National University, ernestryu@snu.ac.kr

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MS73

Interactions of Matrix Shape, Coherence, and Rank on Matrix Completion

In this project, we explore matrix completion for recommender systems. Using synthetic data and real datasets such as Amazon, Netflix, MovieLens, we draw the relations among matrix coherence, rank, and regularization models in order to understand matrix recovery. We observe that the most-squared matrix tends to give the highest accuracy for matrix completion via nuclear norm minimization, which can be justified by matrix coherence. Most matrix completion techniques rely on singular value decomposition (SVD). We find that an approximated scheme of SVD is not only faster but also better than the standard SVD. Lastly, we discover that the transform L_1 model achieves the best matrix recovery results among some existing approaches such as nuclear norm and L_p Schatten norm. Faculty Advisors: Dr. Lou, Yifei, University of Texas at Dallas

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MS73

Numerical Computation of the Tracy-Widom Distribution

Recently, random matrix theory has become one of the most exciting fields in probability theory, and has been applied to problems in high dimensional data analysis, wireless communications, finance, etc. The Tracy-Widom distribution, describing the normalized largest eigenvalue of a random Hermitian matrix, is one of the most important probability distributions in random matrix theory. In the first half of the talk, we will give an overview of existing numerical methods for evaluating the Tracy-Widom distribution, including methods based on solving an ordinary differential equation, and approximating a Fredholm determinant. In the second half of the talk, we will give an introduction to a new method, which also approximates a Fredholm determinant, and is based on exploiting a pair of commuting differential and integral operators. Our new method evaluates the distribution to full absolute precision everywhere rapidly, including in both tails. Moreover, it evaluates the right tail of the distribution to full relative precision. Faculty Advisors: Kirill Serkh, Department of Mathematics at University of Toronto, kserkh@math.toronto.edu

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MS73

Automated Computer Discovery of Geometric Theorems

We introduce a new feature to the online GeoGebra Math App called the Discover Command. The Discover Command is implemented through an open-source Java extension that analyzes Euclidean geometric figures, identifies their salient patterns and properties, determines relevant theorems, proves them symbolically, and reports these findings to the user. GeoGebra translates the geometric setup into an algebraic equation system and uses Grbner bases to determine whether a statement is always true, generally true, partially true, or false. We discuss algorithms used in the Discover Command, including identification of congruent segments, parallel lines, collinear points, concyclic points, parallel lines, and perpendicular lines. We demonstrate the capabilities of the Discover Command computations to a 20-gon, Eulers line, the nine-point circle, as well as proofs of Brahmaguptas theorem, Napoleons theorem, and Thebaults first two theorems. We discuss the mathematical strategies to optimize the scope of the analysis and avoid combinatorial explosion. Applications to education, geometric discovery and exploration, and upper level mathematics are reviewed. Faculty Advisors: Kovcs, Zoltn, Private University of Education, Diocese Linz, zoltan.kovacs@ph-linz.at

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MS74

Coordination and Symmetry-Breaking in Cilia and Flagella

Biological microfilaments, such as cilia and flagella, exhibit a variety of synchronization modes. As the surrounding fluid is an obvious medium for force transmission, hydrodynamic interactions are deemed crucial for synchronization. Two flagella coupled via the fluid medium only have been shown to synchronize their beating in phase or antiphase at close interflagellar distance. Synchronized states with non-trivial phase lags have also been observed. Here, we use an elastohydrodynamic filament model in conjunction with numerical simulations and a Floquet-type theoretical analysis, to demonstrate that it is possible to reach multiple synchronization states by varying the intrinsic activity of the filament and the strength of hydrodynamic coupling between the two filaments. Then, through derivation of reduced-order evolution equations for the phase difference between the filaments at weak coupling, and using a Kuramoto-style phase sensitivity analysis, we reveal the nature of the bifurcations underlying transitions between different synchronized states, especially states with broken symmetry.

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MS74

Hydrodynamical Coupling of Flagella on a Spherical Body

Flagella are hair-like appendages attached to microorganisms that allow the organisms to traverse their fluid environment. The algae Volvox are phototactic, spherical swimmers with thousands of biflagellate somatic cells embedded in their surface. Their flagella coordinate their beating, which leads to forward swimming with slight rotations; the coordination of their flagella is not fully understood. In this work, we extend a previously published mathematical model of coordinated flagella on a flat surface to study coordination on the exterior surface of a sphere. The goal was to determine if factors related to the spherical shape affected flagellar synchronization. Each beating flagella itself is modeled as a small rotating sphere, attached to a point just above the spherical surface by a spring, and the effects of all other flagella are accounted for with a regularized image system for Stokes flow outside of a sphere. We consider flagellar beating in meridional planes with slight offsets and from the anterior to posterior pole. We found that this minimal model can achieve large-scale coordination of flagella that leads to metachronal waves and also results in velocity fields that represent forward swimming with rotation. We varied parameters for meridional offsets, spring stiffness and number of flagella to study how they each affected the coordination.

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MS74

A Computational Approach to Simulate Microswimmers Propelled by Bacterial Flagella

Peritrichously flagellated bacteria swim in a fluid environment by rotating motors embedded in the cell membrane and consequently rotating multiple helical flagella. We present a novel mathematical model of a microswimmer that can freely run propelled by a flagellar bundle and tumble upon motor reversals. Our cell model is composed of a rod-shaped rigid cell body and multiple flagella that are randomly distributed over the cell body. These flagella can go through polymorphic transformations. We demonstrate that flagellar bundling is influenced by random distribution of flagella and the number of flagella. Moreover, reorientation of cells is affected by the number of flagella, how many flagella change their polymorphisms within a cell, when the tumble time starts, and different combinations of polymorphic sequences. Our new method can simulate numerous types of microorganisms and may help to understand their characteristic swimming mechanisms.

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MS74

Viscoelastic Network Remodeling by Microswimmers

Microorganisms often navigate a complex environment composed of a viscous fluid with suspended microstructures such as elastic polymers and filamentous networks. These microstructures can have similar length scales to the microorganisms, leading to complex swimming dynamics. Some microorganisms are known to remodel the viscoelastic networks they move through. In order to gain insight into the coupling between swimming dynamics and network remodeling, we use a regularized Stokeslet boundary element method to compute the motion of a microswimmer consisting of a spherical body and rotating helical flagellum. The viscoelastic network is represented by a cloud of points with virtual Maxwell element links. We consider two models of network remodeling in which (1) links break based on their distance to the microswimmer body, modeling enzymatic dissolution, or (2) links break based on a threshold tension force. We compare the swimming performance of the microbes in each remodeling paradigm as they penetrate and move through the network.

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MS75

Sparse Nonlinear Models of Flow Physics from Data

Many tasks in fluid mechanics, such as design optimization and control, are challenging because fluids are nonlinear and exhibit a large range of scales in both space and time. This range of scales necessitates exceedingly high-dimensional measurements and computational discretization to resolve all relevant features, resulting in vast data sets and time-intensive computations. Indeed, fluid dynamics is one of the original big data fields, and many high-performance computing architectures, experimental measurement techniques, and advanced data processing and visualization algorithms were driven by decades of research in fluid mechanics. Machine learning constitutes a growing set of powerful techniques to extract patterns and build models from this data, complementing the existing theoretical, numerical, and experimental efforts in fluid mechanics. In this talk, we will explore current goals and opportunities for machine learning in fluid mechanics, and we will highlight a number of recent technical advances. Because fluid dynamics is central to transportation, health, and defense systems, we will emphasize the importance of machine learning solutions that are interpretable, explainable, generalizable, and that respect known physics.

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MS76

Extreme Superposition: High-Order Rogue Waves in the Far-Field Regime

It is known from our recent work that both fundamental rogue wave solutions (with Peter D. Miller and Liming Ling) and multi-pole soliton solutions (with R. Buckingham) of the nonlinear Schrdinger (NLS) equation exhibit the same asymptotic behavior in the limit of large order near the peak amplitude point, despite the quite different boundary conditions these solutions satisfy at infinity. In this work, we place solitons and rogue wave solutions in a single continuum family of solutions of the NLS equation parametrized by a positive real parameter M, whose different quantizations give rogue waves and solitons, in which case M becomes correlated with the order of these special solutions. We show that the above-mentioned similar asymptotic behavior in fact extends to a large region of the space-time, expanding in size as $M \to +\infty$ at a rate proportional to M. Within this region, the large-M asymptotic behavior of solutions is rather insensitive to any particular choice of specific unbounded and increasing sequence of values of M. On the other hand, in the complementary region one sees qualitatively different asymptotic behavior along different sequences.

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MS76

Local Solutions to Completely Integrable Partial Differential Equations

More than a century ago, Whittaker developed a theory of the 3D Laplace equation and the (2+1)D wave equation based on a general expression of the local solutions. This theory was eclipsed by more general methods of linear PDEs, but at the time it provided a powerful tool for analysis. For completely integrable nonlinear PDEs, a general expression of the local solutions is still a work in progress. The nonlocal dbar problem dressing method of Zakharov and Manakov (based on the approach of Ablowitz, Bar Yaacov, and Fokas to the IST for the KP equation) provides a candidate for a general expression of the local solutions to completely integrable systems. In this talk I will describe some recent results that give evidence that nonlocal dbar problem dressing method has the potential to provide a general local theory of real solutions to the KdV equation, and I will describe a framework to pursue analogous results for the KP equation. I will also discuss some numerical experiments based on this theory, and potential avenues for further asymptotic analysis. This talk will involve collaborations with Dmitry Zakharov and Vladimir Zakharov.

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MS76

Three-Dimensional Waves under Ice in Various Regimes Computed with Novel Preconditioning Methods

In this talk, we present solutions to the three-dimensional Euler equations describing travelling waves under an ice sheet. Reformulating the equations using a boundary-integral method, we solve the resulting equations based on a Newton-Krylov method, employing a novel preconditioning technique. Using elastic plate theory, we examine solutions for a variety of conditions at the boundary such as waves generated by different pressure distributions and the effect varying thickness of ice has on wave propagation. We show that even under these different conditions, our preconditioning methods are efficient and allow us to increase the grid refinement and decrease the run-time of our computations in comparison to previous methods.

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MS77

Experiments on Upper Hessenberg and Toeplitz Bohemians

We look experimentally at Bohemian matrices, primarily those with entries from $\{-1, 0, +1\}$. More, we specialize the matrices to be upper Hessenberg, with subdiagonal entries 1. We also examine subfamilies of these families. Many properties remain after these specializations, some of which surprised us. We count stable matrices, normal matrices, and neutral matrices, and tabulate the results of our experiments. We generate a list of conjectures from our experiments; some of these conjectures have now been proved, but others remain open.

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MS77

Putting Skew-Symmetric Tridiagonal Bohemians on the Calendar

This talk is intended as a light-hearted introduction to Bohemian Matrices and some of their applications, in preparation for the rest of the minisymposium. A Bohemian Matrix family is a set of matrices, usually structured in some way, all of whose entries come from a bounded (usually finite and thus discrete) population. This idea is a useful specialization in the sense of Plya: by restricting the class of entries, we may be able to discover and prove something useful. In this talk I will look at *skew-symmetric tridiagonal* matrices with entries from such populations as $\{1 \pm i\}$; if the dimension of the matrix is m, then there are precisely 2^{m-1} such matrices. The symmetries of the eigenvalues include negation and conjugation, however, and so a density plot of all the eigenvalues of all matrices of dimension (say) 22 has a pleasing appearance, enough so that I put it on a calendar (available at bohemianmatrices.com, though not so useful in July as it is at this time of writing). But at dimensions 7, 15, and 31 there are surprises; we will talk about what we can learn from these pictures, and what we can prove.

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MS77

Determinants of Normalized Bohemian Upper Hessenberg Matrices

A matrix is Bohemian if its elements are taken from a finite set of integers. A upper Hessenberg matrix is normalized if all its subdiagonal elements are ones, and hollow if it has only zeros along the main diagonal. All possible determinants of families of normalized and hollow normalized Bohemian upper Hessenberg matrices are enumerated. It is shown that in the case of hollow matrices the maximal determinants are related to a generalization of Fibonacci numbers. Several conjectures recently stated by Corless and Thornton follow from these results.

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MS77

Eigenvalues of Magic Squares and Related Bohemian Matrices

Magic squares are a special class of BOunded HEight Matrices with Integer entries. This talk is about the spectrum of magic squares generated by MATLAB's eig() command for doubly even and odd dimensions. Interestingly, the odd magic squares are related to g-circulant matrices. The g-circulant is a matrix with every row being a g-cyclic shift of the previous row. We further explore the spectra of g-circulant matrices and diagonally scaled permutation matrices.

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MS78

On Stability of Deep Neural Network-Based Models

In this talk, we present a dynamical systems perspective on deep neural networks (DNNs). As a base, we leverage the equivalence of neural networks with parameter-varying affine maps parameterized by the state (feature) vector, which allows us to apply a range of analysis methods from linear systems theory. In particular, we focus on the operator norms and provide sufficient conditions for the stability of DNNs via Banach fixed point theorem. We expose links between the operator norms of layer-wise weight parametrizations, different activation functions, and their effect on the stability of the network's dynamics. As a next step, we propose a natural extension of the deterministic stability conditions of DNNs to stochastic stability in the context of Deep Markov models (DMM). DMMs are popular generative models that use neural networks to parametrize the transition of Markov probability distributions. However, the fundamental stochastic stability guarantees of such models have not been thoroughly investigated. We demonstrate that constraints on the operator norms of the layer weights and careful choice of the activation functions lead to guaranteed stability of models based on deep neural networks. We empirically substantiate our theoretical results via several tutorial numerical experiments.

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MS78

Data-Driven Framework for Decision and Control of Dynamic Systems

In many engineering and scientific research areas, analyses, simulations and optimizations of complex systems have been objectives of many past research efforts. One of the fundamental challenges of complex system modeling and control, which is that high-fidelity ab initio models can be prohibitively expensive to construct. This limitation is not necessarily due to the lack of fundamental understanding of the underlying natural phenomena but due to practical constraints, such as the difficulties in instrumenting the complex systems to collect relevant data, the need to resolve inherent uncertainties in the models (e.g., due to unmodeled physics), and the loss of observability due to excessive exogenous noise. In this talk, we will present a high-level overview of the collaborative project Data-Driven Decision Control for Complex Systems (DnC2S), and provides an overview to bring together the various topics featured in this two-part minisymposium.

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MS78

A Reliable Feature Extraction Approach for Real-Time Processing and Analytics of Neutron Scattering Data

The efficiency and reliability of extracting meaningful features from neutron scattering data generated in an experiment is critical to the design of follow-up experiments. Unfortunately, due to the unreliability of existing data analytics tools, instrument scientists often need to manually analyze large amount of scattering data after each experiment, which usually delays progress of users programs. To alleviate such challenge, exploiting our recent achievements on UQ for ML, we developed a reliable algorithm for feature extraction and demonstrated its performance on extracting the Bragg peak feature from neutron diffraction data. Specifically, our approach introduces ensemble UQ method into R-CNNs to detect and extract Bragg peaks from diffraction data. We demonstrated that our method achieves similar accuracy as manual analysis but significantly improves the efficiency. More importantly, the confidence score associated with each detected feature can correctly indicate out-of-distribution (OOD) data by assigning low confidence scores to data shifted from training data, while the current R-CNN model often provides overconfident scores for OOD data.

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MS78

Overview of Drivers for AI-Informed Decision and Control in Energy Applications

The need for modeling, controlling, and optimizing complex systems arises often in energy generation, distribution, and end-use applications. An illustrative list of examples includes building energy optimization, automatic/autonomous control of electrical and process heat generation in fossil and nuclear plants, high-energy user facility operations and control, and resource allocation in high-performance computing systems. Recent research in this area has focused on developing the mathematical foundations and framework for controlling and optimizing complex systems through data-driven machine learning and artificial intelligence (AI). Although these complex systems have generally had a history of robust control and operations, challenges from an application perspective include surrogate system model development and updates from data, accounting for uncertainties in data and model predictions, and learning optimal control policies. This talk describes the application drivers for research described in other presentations in this mini-symposium, on the mathematical framework for AI-informed decision and control using probabilistic graph models and neural network models. The applications drivers discussed here were selected based on availability of the curated data, existing (baseline) solutions for control and optimization, and—to a lesser extent—the availability of physical or surrogate models that are expected to be of use in PGM and NN model construction and evaluation.

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MS79

Using the Tools of Machine Learning to Accelerate Data Assimilation in Experiments

I will discuss two examples of experimental collaborations we have been carry out that aim to use the tools of machine learning to accelerate data assimilation in experiments. The first example involves taking 2d slices of a fluid flow, in which there is particle image velocimetry in each slice. We aim to take different slices and together with the equations of motion (the Navier-Stokes equations) reconstruct the entire 3d flow. In the second project, we try to infer particle tracks in dense colloidal suspensions. Experiments use confocal microscopy to find the location of the particles in the individual frames. We explore different algorithms for reconstructing the track of each particle at high resolution.

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MS79

Data-Free and Data-Driven Uncertainty Quantifi-

cation in Turbulent Flow Simulations

Despite continued advances in high-fidelity turbulent flow simulations, closure models based on the Reynolds-Averaged Navier-Stokes (RANS) equations are projected to remain in use for considerable time to come. However, it is common knowledge that RANS predictions are corrupted by epistemic model-form uncertainty to a degree which is unknown a-priori. Hence, to obtain a computational framework of predictive utility, a model-form Uncertainty Quantification framework is indispensable. Applying the spectral decomposition to the modeled Reynolds-Stress Tensor (RST) allows for the introduction of decoupled perturbations into the baseline intensity (kinetic energy), shape (eigenvalues), and orientation (eigenvectors). Within this perturbation framework, we look for a-priori known limiting physical bounds. Since these bounds are universal, they can be used to constrain uncertainty estimates in any predictive flow scenario. Thus, even in the absence of relevant training data, we can maximize the spectral perturbations in order to obtain conservative uncertainty intervals. On the other hand, any high-fidelity reference data can be used to further constrain the uncertainty estimates using commonly available data assimilation techniques. We will demonstrate our framework on canonical flow problems using random forest regression and deep neural networks to incorporate DNS data into the uncertainty estimates of conventional RANs closures.

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MS79

Deep Learning-Based PDE Augmentation for Large-Eddy Simulation

Standard applications of deep learning methods to physics can be considered *ad hoc* in the absence of governing laws, which are typically most completely stated as systems of PDEs. We introduce a framework that leverages as much *a priori* known physics as possible by embedding deep neural networks in PDE systems and optimizing them over the (possibly unsteady) solutions. In this manner, the solution itself is the training target, rather than the simple mismatch between the model and a-priori unclosed terms such as the Reynolds-stress tensor for Reynolds-averaged NavierStokes (RANS) formulations or the subgrid-stress tensor for large-eddy simulation (LES). The framework augments the spatio-temporally averaged (RANS) or coarse-grained (LES) PDEs by accounting for dynamical discrepancies between these and the trusted PDE solution. The method is applied to the closure of the LES governing equations. Filtered (LES) and averaged (RANS) velocity fields, obtained from direct numerical simulation (DNS), serve as training and out-of-sample prediction targets. Applications are demonstrated in isotropic turbulence, turbulent jets, and turbulent wakes. The model is found to identify dynamically important asymmetries that are unsupported by symmetric subgrid-stress models. Extensions are made to turbulent combustion and high-speed flows.

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MS79

Multi-Fidelity Bayesian Neural Networks for Inverse Problems with Noisy Data

We propose a new class of Bayesian neural networks (BNNs) that can be trained using noisy data of variable fidelity, and we apply them to learn function approximations as well as to solve inverse problems based on partial differential equations (PDEs). These multi-fidelity BNNs consist of three neural networks: The first is a fully connected neural network, which is trained following the maximum a posteriori probability (MAP) method to fit the low-fidelity data; the second is a Bayesian neural network employed to capture the cross-correlation with uncertainty quantification between the low- and high-fidelity data; and the last one is the physics-informed neural network, which encodes the physical laws described by PDEs. Specifically, we first approximate a one- and four-dimensional function, and then infer the reaction rates in one- and two-dimensional diffusion-reaction systems. Moreover, we infer the sea surface temperature (SST) in the Massachusetts and Cape Cod Bays using satellite images and in-situ measurements. Taken together, our results demonstrate that the present method can capture both linear and nonlinear correlation between the low- and high-fidelity data adaptively, identify unknown parameters in PDEs, and quantify uncertainties in predictions, given a few scattered noisy high-fidelity data. Finally, we demonstrate that we can effectively and efficiently reduce the uncertainties and hence enhance the prediction accuracy with an active learning approach.

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MS80

Breathers in Hexagonally Packed Magnetic Lattices

This talk concerns breathers, which are temporally periodic and spatially localized structures, in a two-dimensional array of repelling magnets. In particular a lattice with a hexagonal configuration with a light-mass defect is considered. Using a damped, driven variant of a vector FermiPastaUlamTsingou lattice we find good qualitative agreement between theory and experiments for a variety of dynamical behaviors. Bifurcations that result from variation of the drive amplitude, angle, and frequency will be discussed as well as quasi-periodic dynamics.

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MS80

Long Wave Nanopterons in Dimer Fermi-Pasta-Ulam-Tsingou Lattices via Spatial Dynamics

Mass and spring dimer Fermi-Pasta-Ulam-Tsingou (FPUT) lattices are known to possess nanopteron traveling wave solutions to their equations of motion in the long wave limit, close to suitably scaled KdV solitary waves. These are traveling waves whose profiles asymptote to small periodic oscillations at spatial infinity. Just how small are these oscillations? Can their amplitudes ever be zero? How about exponentially small in the relevant small parameter, or just algebraically small? And what happens to the behavior of the original position coordinates of the lattice, since these traveling wave results are known only in relative displacement coordinates? Using results and techniques from spatial dynamics and center manifold theory (and nontrivial modifications and corrections thereof), we will answer these questions.

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MS80

Stability of Traveling Waves in a Driven Frenkel-Kontorova Model

In this work we revisit a classical problem of traveling waves in a damped Frenkel-Kontorova lattice driven by a constant external force. We compute these solutions as fixed points of a nonlinear map and obtain the corresponding kinetic relation between the driving force and the velocity of the wave for different values of the damping coefficient. We show that the kinetic curve can become *non-monotone* at small velocities, due to resonances with linear modes, and also at large velocities where the kinetic relation becomes *multivalued*. Exploring the spectral stability of the obtained waveforms, we identify a criterion for instability of the traveling wave solutions: monotonically decreasing portions of the kinetic curve always bear an unstable eigendirection. Our stability results are corroborated by direct numerical simulations which also reveal the possible outcomes of dynamical instabilities.

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MS80

Breathers As Metastable States for Weakly Damped Lattices of Hamiltonian Oscillators

We discuss the flow of energy in a lattice of Hamiltonian oscillators with weak damping at one end of the lattice. We derive bounds on the rate of dissipation when the initial energy in the lattice is localized in a spatially distant part of the lattice. For a special model, we exhibit a family of breather solutions for the undamped problem and show that the rate of energy dissipation can be explained by a very slow drift along this family of breathers. This is joint work with No Cuneo (Univ. of Paris 7), Jean-Pierre Eckmann (Univ. of Geneva) and Daniel Caballero (Boston Univ.)

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MS81

On the Spatial and Temporal Order of Convergence of Partial Differential Equations

In this talk, I will discuss the leading order terms of the local truncation error of hyperbolic and parabolic partial differential equations (PDEs). In the asymptotic regime, where the local truncation error is dominated by the powers of the grid-spacing and the time-step rather than their coefficients, we make the following observations. The order of convergence of stable numerical solutions of hyperbolic or parabolic PDEs at constant ratio of time-step to grid-spacing is governed by the minimum of the orders of the spatial and temporal discretizations. If refinement is performed only in space or time, convergence cannot even be attained. Our theory is independent of the order of spatial and temporal discretizations, and applies to any hyperbolic or parabolic PDE, be it linear or nonlinear, and employing finite difference, finite volume or finite element discretization in space, and advanced in time with a predictor-corrector, multi-stage or a deferred correction method. If the PDE is reduced to an ordinary differential equation (ODE) by specifying the spatial gradient(s) of the dependent variable and the coefficients and the source terms to be zero, then the standard local truncation error of the ODE is recovered. A number of numerical experiments are performed to demonstrate our theoretical findings.

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MS81

Paralpha: a Parallel-in-Time and Space PDE Solver

Parallel-in-Time algorithms for hyperbolic problems often encountered in physics are notoriously difficult to design, even for linear problems. In this talk, we propose a new parallel-in-time iterative method for solving linear composite collocation problems, even those stemming from hyperbolic PDEs. These composite collocation problems are typically the basis for the multi-level PFASST algorithm. In contrast to PFASSTs multi-level approach which may cause problems when it comes to hyperbolic problems, we use a single-level preconditioned Richardson iterations with a near-circulant preconditioner that can be diagonalized using fast Fourier transformations in time. As a consequence, we obtain time-interval decoupled problems in each iteration which we propose to solve directly in parallel across the collocation nodes, using a diagonalization of the slightly modified quadrature matrix arising from the Runge-Kutta propagation. This brings us to a doubly parallel-in-time method called Paralpha which solves linear problems very efficiently. Using fast Fourier transformations in time on the preconditioner, the communication becomes very efficient and there is no need to worry about coarsening strategies. We present theoretical and practical convergence and performance results as well as strengths and weaknesses of this method.

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MS81

Highly Accurate and Flexible Multirate Time-Stepping Methods for Multiphysics Applications

Dynamics of varying time scales are a staple in simulations of multiphysics scientific applications. In order to resolve these different time scales, multirate methods use different optimal time steps and algorithms for the slow and fast dynamics. Of recent interest are methods for which the fast solution is propagated between slow stages through the solution of modified initial value problems. We refer to such methods as multirate infinitesimal (MIS) type methods. In this talk, we discuss our recent work in constructing MIS-type methods that are high order and flexible. Our new approaches include methods with IMEX treatment of the slow dynamics, integration of the fast dynamics with any scheme of sufficient order, and multirate schemes with up to sixth order convergence. We present numerical results on convergence and efficiency and compare our methods with other well-known MIS-type methods.

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MS81

Integration of the Lorentz Equations with Boris Spectral Deferred Corrections (Boris-SDC)

The Boris integrator is one of the most popular time stepping method for solving the Lorentz equations. We will introduce a new time stepping method with arbitrary order of accuracy that combines Boris' method with spectral deferred corrections (SDC) as well as ideas from the GMRES iterative linear solver. We will show performance results for the resulting Boris spectral deferred correction method (Boris-SDC) when tracking fast ions in the equilibrium magnetic field of the DIIID and JET fusion reactor. Furthermore we will describe a modification to make the method work for the relativistic case and show some results when it is used as particle pusher in a particle-in-cell code.

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MS82

RDMA-Based Sparse Matrix Multiplication on GPUs

Sparse matrix multiplication is an important kernel for large-scale graph processing as well as a host of other data-intensive applications. As GPUs become more dominant in both data centers and supercomputers, it is crucial to capitalize on new network technologies, such as GPUDirect RDMA, as well as new asynchronous algorithms that allow for better strong scaling. In this talk, we examine RDMA-based data structures and algorithms for implementing sparse matrix multiplication on GPUs, including both sparse-times-dense (SpMM) and sparse-times-sparse (SpGEMM). We explore asynchronous algorithms, as well as work-stealing algorithms, that allow for better scaling, and demonstrate how they can outperform state-of-the-art bulk synchronous algorithms.

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MS82

Chapel: An Example of Language Level PGAS Support

Programs that involve data intensive computations should carefully distribute the data and computation on the available computer system. This is easier to do when working with programming abstractions that support a Partitioned Global Address Space, as demonstrated by the Chapel programming language. From explicit control over the node where an operation will run via the locale type and on statements, to the use of different distributions for an array that determine where its contents are located in memory, Chapels multi-resolution design allows users to take as active or as passive a role as desired in distributing their data. Chapel also handles the communication necessary for accessing the distributed data, minimizing the potential for user errors and enabling compiler optimizations that would not be possible in a library-based solution. Using Chapels variable representation of index sets (known as domains) and the optional extension that allows them to be distributed (known as domain maps), the same Chapel executable can be run over varying numbers of nodes without having to recompile the program. And swapping to different distribution strategies for experimentation during development is as simple as changing a line of code. This talk will go into all of these language features and their uses, illustrating some of the productivity and performance benefits with code snippets and performance results.

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MS82

Graph Algorithms in PGAS: Runtime vs Language Support

The Partitioned Global Address Space (PGAS) programming model has been proposed as an alternative to the message-passing programming model, that can be implemented either as a runtime or a programming language. Targeting both productivity and performance, efficient execution of irregular applications such as graph algorithms require additional support from the PGAS model. In particular, the following aspects are important: message coalescing, termination detection, better support for overlapping communication and computation with messaging primitives, lightweight tasking/threading, and active message support. Replacing existing two-sided communication usage in graph application codes with PGAS models in a manner that fully exploits the benefit of these programming models may require nontrivial development efforts, but offers interesting prospects for enhancing the expressiveness and composability of graph applications. In this talk, we will briefly discuss our experience with implementing graph algorithms in various PGAS/Pseudo-PGAS runtimes and programming languages: Indiana Universitys AM++ runtime, Berkeleys UPC++, Indiana Universitys HPX-5 runtime, PNNLs ARTS runtime and CRAY/HPEs Chapel programming language and MPI RMA. We will also discuss some of the strategies and incentives to transform two-sided graph applications such as clustering and matching to a one-sided model, particularly in the context of MPI-3 RMA and UPC++.

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MS82

The Global Arrays Toolkit: A PGAS Programming Library

We will provide a brief overview of the Global Arrays (GA) Toolkit and discuss the underlying runtimes. GA provides an abstraction for creating large arrays distributed across multiple processors that can be accessed using simple, one-sided shared memory style semantics. GA supports put/get/accumulate operations that can be used to access data from anywhere in the array without coordinating directly with the processors holding the data. This can greatly simplify the implementation of many parallel algorithms. This talk will provide a description of available GA runtimes, basic GA operations and current work to extend GA to GPUs.

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MS83

Stability of Traveling-Wave Solutions to a Family of Bidirectional Whitham Systems

The Whitham equation is a model for the evolution of unidirectional waves on shallow water. Aceves-Sanchez et al. (2012) and Hur & Pandey (2018) proposed different bidirectional generalizations of the Whitham equation. Although these systems have been shown to accurately predict the evolution of waves of depression in the laboratory, it is unknown if these systems are well-posed. The Aceves-Sanchez system has been proven to be well-posed in the nonphysical case where the surface displacement is never nonpositive. Numerical simulations of both systems show some characteristics of ill-posedness. The goal of the current work is to study the stability of traveling-wave solutions to a family of bidirectional Whitham systems in hopes of gaining a deeper understanding of their well-posedness.

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MS83

Soliton Dynamics in the Korteweg-de Vries Equation with Nonzero Boundary Conditions

Inspired by recent experiments, the Korteweg-de Vries equation with nonzero Dirichlet boundary conditions is considered. Two types of boundary data are examined: step up (which generates a rarefaction wave) and step down (which creates a dispersive shock wave). Soliton dynamics are analytically studied via inverse scattering transform and a small dispersion asymptotic approximation. Depending on the initial position and amplitude, an incident soliton will either transmit through or become trapped inside a step-induced wave. A formula for the transmitted soliton and its phase shift is derived. The asymptotic approximation provides a description of the trapped soliton dynamics.

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MS83

Unstable Water Waves: A Periodic Evans Function

Approach

I will discuss a new periodic Evans function approach for cylindrical domains, and an application to the spectral instability of Stokes waves. Numerical evidence suggests instability whenever the unperturbed wave is 'resonant' with its infinitesimal perturbations. This has not been studied analytically except the Benjamin-Feir instability, near the origin of the spectral plane, when (wave number)x(depth)¿1.3627.... I will discuss an alternative proof of the Benjamin-Feir instability and, also, the first proof of spectral instability away from the origin when 0.86430...¡(wave number)x(depth)¡1.00804..., elucidating numerical findings. I will remark about extensions to capillary-gravity waves and Stokes waves in a constant vorticity flow.

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MS83

Shock Wave Stabilization in Superfluids with Higher-Order Dispersion

Ultracold atomic gases are highly adaptable platforms that can be used to investigate a variety of superfluid hydrodynamic features. Over the last decade, a particularly flexible tool has been developed that provides researchers the ability to modify a systems dispersion such that regions of higher-order dispersive terms emerge. Using an elongated Bose-Einstein condensate, we induce spin-orbit coupling by coherently coupling two spin states, which breaks Galilean invariance. We then experimentally probe the system using a pulsed attractive optical potential. We show the observed dynamics diverge from those found in past experiments due to the interaction of emerging vorticity and the governing dispersion in the system, which leads to a stabilized traveling shock front in the region of higher-order dispersion. The results of our experiments establish ultracold atomic gases as a platform for discovering new varieties of hydrodynamic shock features in regions with higher-order dispersion and open the door to a new era of quantum shock wave studies. We recognize support and funding from the NSF under Grant No. PHY-1607495 and PHY-1912540.

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MS84

Mathematical Modelling of Salmonella-Infected Red Onions using Markov Processes

The consumption of Salmonella-infected produce has been an alarming issue to human health after numerous reports of Salmonellosis outbreaks linked to red onions have been reported by the CDC in 2020. Hence, a mathematical model that examines the growth of red onions with potential exposure to the foodborne pathogen is necessary in gaining insights on how the bacteria can be contained at the farm-level to mitigate human health risks. In particular, we employ Markov processes to model the mechanism that simulates the dynamics of Salmonella pathogens in onions. We later found that irrigation water is the pathogens most likely transmission route onto the onions. Thus, we provide agricultural advice by proposing recommendations on how frequent irrigation water sources should be cleaned in reducing substantial amounts of Salmonella concentration while minimizing cleaning costs. On average, irrigation water tanks should be cleaned every 2-7 days based on the results of our simulations. Through our research study, we desire to see less cases reported, should another massive outbreak of Salmonella-infections linked to fresh produce such as in red onions happen in some foreseeable future. Faculty Advisors: Moyles, Iain, York University, imoyles@yorku.ca

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MS84

Modeling Chytridiomycosis Disease and its Thermal Acclimation within a Frog Population

Batrachochytrium dendrobatidis is a pathogenic fungus implicated in the global decline of amphibians. Several studies suggest that temperature plays a significant role in Batrachochytrium dendrobatidis and a frog's development. However, there are many questions unanswered regarding these interactions. To investigate the effect of temperature dependency on the disease dynamics, we developed a mathematical model with vital rates of both the fungus and frogs depending on temperature. We utilized parameter estimation to compute and fit the model to different regions and show the decimation impact of the frog population. Our simulation results corroborate with literature studies showing the correlation between temperature and chytridiomycosis disease. Moreover, Our results suggest that temperature plays a major role in the life history of frogs and in disease dynamics. Furthermore, our results suggest critical intervention strategies that can be utilized to mitigate the disease within frog populations. Faculty Advisors: Vinodh Chellamuthu, Dixie State University, Vinodh.Chellamuthu@dixie.edu

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MS84

Modeling the Impact of Wolbachias Transinfection and its Effectiveness on Mitigating the Spread of Dengue

Dengue fever is one of the worlds most common viral-borne diseases, its spread is most prominent in tropical and subtropical climates. The infection is caused by bites from mosquitoes carrying the disease and a secondary infection can lead to severe dengue fever. The cycle of transmission can be broken by using Wolbachia, a bacterium shown to reduce levels of dengue virus in the mosquito, shorten the host mosquitos lifespan, and cause reproductive abnormalities in the host. We develop a mathematical model using a system of nonlinear ordinary differential equations that incorporate Wolbachia transinfection to study the epidemiologic trends of two viral dengue serotypes. Moreover, our model considers temporary cross-immunity within the two serotypes and the impact of temperature dependency on mosquitoes' vital rates. Our simulation results suggest the introduction of Wolbachia carrying mosquitoes at optimal times can decrease the number of dengue transmitting vectors and, consequently, reduce the frequency and prevalence of outbreaks. Faculty Advisors: Chellamuthu, Vinodh, Dixie State University, vinodh.chellamuthu@dixie.edu.

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MS84

Mathematical Modeling of U.S. Elections Dynamics

Forecasting the outcomes of U.S. elections is a relevant and complex task that has been approached in many ways, often incorporating statistical or political-science methods. We take a differential-equations approach to forecasting elections by applying a prior compartmental model for the evolution of voting intentions. The model accounts for two types of dynamics: the spread of Democratic or Republican voting intentions between states, and the turnover of committed voters to undecided ones. The model parameters are determined based on polling data, and simulations are run in MATLAB. Through thousands of simulated elections with our stochastic differential equations, we forecast a range of election outcomes at the state level. The models final forecasts for past presidential, senatorial, and gubernatorial elections are comparable to those of popular forecasting sites like FiveThirtyEight. We have examined how the accuracy of the models forecasts of past elections changes in time as we approach each election day, and applied the model to create forecasts of the 2020 U.S. elections. Leading up to the 2020 elections, we continuously posted forecasts with visualizations on a website that we created. We will discuss our 2020 election forecasts, our work on visualizing uncertainty, and our efforts to improve the accuracy of the model by weighting the polling data in different ways. Faculty Advisors: Volkening, Alexandria, Northwestern University, alexandria.volkening@northwestern.edu

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MS84

Optimal Control of Algae Biofilm Growth in Wastewater Treatment using Computational Mathematical Models

Microalgal biofilms are comprised of a syntrophic consortium of microalgae and other microorganisms embedded within an extracellular matrix. Despite significant processes in the application of microalgal biofilms in wastewater treatment, mechanistic understanding and optimization of microalgal biomass yield and productivity under environmental constraints is still lacking. This paper identifies theoretical insights on this challenging biological problem by leveraging novel mathematical and computational tools. In particular, utilizing a computational mathematical model to advance the understanding of microalgal biofilm growth kinetics under environmental constraints through a systematic parameter study. Moreover, the design of algae biofilm reactors for optimal biomass yield and productivity in wastewater treatment under different environments is explored. The proposed model could be further calibrated to generate reliable predictions that can improve the design, operation, and management of microalgal biofilms in wastewater treatment. Faculty Advisors: Zhao, Jia, Utah State University, jia.zhao@usu.edu

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MS84

A Mathematical Model of COVID-19: Efficacy of Vaccination with Heterogeneous Populations

Infections from the novel coronavirus disease 2019 (COVID-19) remain superfluous as the disease continues to spread profusely across the world. Currently, there is no available vaccine to protect against COVID-19. As scientists work to develop a vaccine, our goal is to explore scenarios for different levels of vaccine effectiveness and varying proportions of vaccinated populations in order to demonstrate the effectiveness of a vaccine in mitigating the spread of COVID-19. We develop a mathematical model to analyze the disease dynamics of COVID-19 in relation to vaccine effectiveness. Furthermore, we performed a data-fitting algorithm to estimate parameters within the model to best resemble current infection trends using data from the Center for Disease Control and Prevention (CDC). We incorporate a vaccinated population and demonstrate the mitigation of COVID-19 with the introduction of a vaccine. Our simulation results determine possible best-case scenarios at varying degrees of vaccine-effectiveness and proportions of vaccinated populations. Moreover, to account for the diseases varying infection and mortality rates based on an individual's age, we further partition the population by age groups to determine which age groups are most vital to vaccinate. Our simulation also identifies the minimal required vaccine efficacy for a given proportion of vaccinated individuals. Faculty Advisors: Chellamuthu,Vinodh,Professor,Vinodh.chellamuthu.dixie.edu

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MS84

Modeling, Analysis, and Control of Student Loan Debt using Epidemiological Models

Student loan debt is a debilitating problem that threatens a large subset of the American population. As of February 2019, the total amount of debt in the U.S. due to student loans amounted to $1.56 trillion. This paper works to mathematically model the student debt situation from the lens of an infectious disease contagion model. The study describes a belief proliferation model. Specifically, the spread occurs through the unfounded external reassurance to students that the value of their college education will amount to a future job that will enable them to pay off their loans in full and on time. Built on the classical SEIR compartmental model of epidemiology, this study analyses the movement of individuals in the study set from the susceptible stage to recovered stage using interconnected differential equations. We additionally consider an enhanced model to study the potential effect of an educational awareness program and the financial strain of the COVID-19 pandemic through respective optimal control variables. Utilizing Pontryagin's maximum principle, the augmented model determines the ideal control value to mitigate the rate of students refinancing their loans when unable to meet the required payments. Faculty Advisors: Seshaiyer, Padmanabhan, George Mason University

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MS84

Advanced Analysis of Hispanic Voter Activity in Florida through Sub-Ethnicities Identification

The aim of this project is to analyze Hispanic voter trends and to categorize each voter into selected sub-groups based on publicly available census data and voter information to then pinpoint which sub-groups need assistance in increasing the overall Hispanic voter turnout. However, public voter information does not include an individuals Hispanic sub-group and Hispanic is a broad term to classify any individual from Latin or South America. Census data was used to help determine the number of Hispanic sub-groups and percentages of individuals within each Hispanic subgroup at a given zip code. The process of identifying an individuals most probable sub-group was determined by creating probability percentages based on their first name, last name(s), and zip code. By calculating percentages of the popularity of a given first name and last name(s) within each of the 19 selected Latin and South American countries, a probability of their sub-group was calculated after combining it with their zip code. After the development of a model and algorithm written in Python, all self-identified Hispanic voters were classified in an effort to analyze Floridas Hispanic Voter trends. This data will help reveal the patterns and behaviors of Hispanic sub-group voting trends for future local and national elections. Faculty Advisors: Berezovski, Mihhail, Embry-Riddle Aeronautical University, berezovm@erau.edu

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MS86

A Force Doublet Model for Bacterial Locomotion in Viscoelastic Environments

In the world of bacterial locomotion, motile organisms generate wakes and eddies that affect their local fluid environment. When many of them are present around each other, they interact with the flows generated by other organisms and form active suspensions whose complex flow structures play a significant role in fluid transport and mixing. In this talk, we present a reduced model for bacterial locomotion that describes their self-propelled motion in a low Reynolds number viscous incompressible fluid. The model is based on a particular limit of regularized Stokeslets with built-in asymmetry in order to produce a swimming direction. The result is a single-particle model of a swimmer that does not require special treatment of the self velocity due to the regularization, while allowing us to efficiently study the collective motion of bacteria. With this model, we are able to model pusher and puller organisms in a straightforward manner for both free-space and periodic domains. We will characterize the particle dynamics and discuss the diffusion of these particles as a function of the concentration density. We will then take advantage of the regularized Stokeslets framework to understand how active suspensions interact with viscoelastic structures, such as biofilms.

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MS86

Ewald Summations for Doubly-Periodic Regularized Stokes Flows Near a Plane Wall

A method is presented for the efficient computation of Stokes flow due to doubly-periodic arrays of regularized forces in 3D near a plane wall. Our approach is based on a variation of Ewald's summation method and the method of images for Stokeslets and regularized Stokeslets. The slowly convergent series resulting from the direct summation of the doubly-periodic array of regularized Stokeslets is recast into the sum of two series, one in real space and one in Fourier space, both having partial sums decaying in a Gaussian manner. The formulation of our method guarantees that the velocity on the wall is analytically zero independent of the number of summands used. We also introduce an empirical approach to compute the 'optimal' number of summands in the real space and Fourier space corresponding to a given splitting parameter.

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MS86

Parallel-in-Time Simulation of Biofluids

We extend Parareal, a parallel-in-time method, to simulate the fluid around bio-inspired, dynamic structures over a period of time. The shapes and positions of the structures can be tracked by solving a system of Ordinary Differential Equations (ODEs). We usually apply an ODE solver to it and invoke a solver for fluid-structure interactions, such as the Method of Regularized Stokeslets (MRS), in the ODE solver to compute the flow field. Parareal aims to accelerate the solution of ODEs by solving them on slices of the time domain simultaneously on multiple processors. It alternates between a "parallel sweep" and a "serial sweep": in the parallel sweep, the solutions on the time slices are predicted simultaneously; and in the serial sweep that follows, a less accurate but faster coarse ODE solver is applied to correct the predicted solutions serially. Our main contributions are demonstrating the applicability of Parareal to the simulation of biofluids, proposing three novel coarse solvers for the serial sweep, and performing convergence analysis for the proposed solvers and for the Parareal equipped with them. The new solvers are constructed by extrapolating existing solvers that use various regularization parameters in the MRS and/or time steps and are easy to implement; they also take advantage of parallel computing. We show that the Parareal equipped with the proposed coarse solvers can achieve a considerably higher parallel speedup than spatial parallelization.

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MS86

Algorithmic Developments for the Method of Regularized Stokeslets

The regularized stokeslet method is an accessible and elegant method for the solution of Stokes flow problems with complex shaped moving boundaries which arise in biological fluid mechanics. This talk will discuss algorithmic developments that preserve the implementational simplicity of the method while significantly reducing computational cost, thereby extending the range of biological systems that can be investigated. Computational approaches include nearest-neighbour interpolation for the traction, which removes the trade-off between regularization and quadrature error, graphical processing unit implementation, and Richardson extrapolation in the regularization parameter. We conclude by discussing applications to sperm motility and the left-right symmetry breaking organ of the vertebrate embryo.

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MS87

Principal Trading Arrangements: Optimality under Temporary and Permanent Price Impact

We study the optimal execution problem in a principal-agent setting. A client contracts to purchase a large position from a dealer at a future point in time. In the interim, the dealer acquires the position from the market, choosing how to split the parent order into smaller child orders. Price impact may have a temporary and a permanent component. There is hidden action in that the client cannot directly dictate the dealer's trades. Rather, she chooses a contract with the goal of minimizing her expected payment, taking as given how the dealer's trading will depend on the contract. Solving the coupled optimization problems of the client and dealer, we characterize explicitly the optimal contract and the dealer's trading strategy.

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MS87

Mortality and Healthcare: a Stochastic Control Analysis under Epstein-Zin Preferences

This paper studies optimal consumption, investment, and healthcare spending under Epstein-Zin preferences. Given consumption and healthcare spending plans, Epstein-Zin utilities are defined over an agent's random lifetime, partially controllable by the agent as healthcare reduces mortality growth. To the best of our knowledge, this is the first time Epstein-Zin utilities are formulated on a controllable random horizon, via an infinite-horizon backward stochastic differential equation with superlinear growth. A new comparison result is established for the uniqueness of associated utility value processes. In a Black-Scholes market, the stochastic control problem is solved through the related Hamilton-Jacobi-Bellman (HJB) equation. The verification argument features a delicate containment of the growth of the controlled morality process, which is unique to our framework, relying on a combination of probabilistic arguments and analysis of the HJB equation. In contrast to prior work under time-separable utilities, Epstein-Zin preferences largely facilitate calibration. In four countries we examined, the model-generated mortality closely approximates actual mortality data; moreover, the calibrated efficacy of healthcare is in broad agreement with empirical studies on healthcare across countries.

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MS87

Mortgage Contracts and Selective Default

We analyze recently proposed mortgage contracts which aim to eliminate selective borrower default when the loan balance exceeds the house price (the "underwater' effect). We show that contracts which automatically reduce the outstanding balance in the event of local house price decline remove the default incentive, but may induce prepayment in low price states. However, low state prepayments vanish if the borrower benefit from home ownership is sufficiently high. We also show that capital gain sharing features, such as prepayment penalties in high house price states, are ineffective, as they virtually eliminate prepayment. For observed foreclosure costs, we find that contracts with automatic balance adjustments become preferable to the traditional fixed rate mortgage at contract rate spreads between 50-100 basis points, depending on how far prices must fall before adjustments are made. Furthermore, these spreads rapidly decrease with the borrower benefit from home ownership. Our results are obtained using American options pricing methods, in a model with diffusive home prices, and either diffusive or constant interest rates. We determine the contract, default and prepayment option values with optimal decision rules. We provide explicit solutions in the perpetual case with constant interest rates; and numerically compute the prepayment and default boundaries in the general setting. This is joint work with Scott Robertston.

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MS87

A Case Study on Stochastic Games on Large Graphs in Mean Field and Sparse Regimes

We study a class of linear-quadratic stochastic differential games in which each player interacts directly only with its nearest neighbors in a given graph. We find a semi-explicit Markovian equilibrium for any transitive graph, in terms of the empirical eigenvalue distribution of the graphs normalized Laplacian matrix. This facilitates large-population asymptotics for various graph sequences, with several sparse and dense examples discussed in detail. In particular, the mean field game is the correct limit only in the dense graph case, i.e., when the degrees diverge in a suitable sense. Even though equilibrium strategies are nonlocal, depending on the behavior of all players, we use a correlation decay estimate to prove a propagation of chaos result in both the dense and sparse regimes, with the sparse case owing to the large distances between typical vertices. We show also that the mean field game solution can be used to construct decentralized approximate equilibria on any sufficiently dense graph sequence, even without assuming that the graphs are transitive.

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MS88

Stein Variational Reduced Basis Bayesian Inversion

We present a Stein variational reduced basis method (SVRB) to solve large-scale PDE-constrained Bayesian inverse problems. To address the computational challenge of drawing numerous samples requiring expensive PDE solves from the posterior distribution, we integrate an adaptive and goal-oriented model reduction technique with an optimization-based Stein variational gradient descent method (SVGD). We present a detailed analysis for the reduced basis approximation errors of the potential and its gradient, the induced errors of the posterior distribution measured by Kullback–Leibler divergence, as well as the errors of the samples. To demonstrate the computational accuracy and efficiency of SVRB, we report results of numerical experiments on a Bayesian inverse problem governed by a diffusion PDE with random parameters with both uniform and Gaussian prior distributions. Over 100X speedups are shown to be achieved while the accuracy of the approximation of the potential and its gradient is preserved.

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MS88

Space and Chaos Expansion Galerkin POD for Uncertainty Quantification of PDEs with Random Parameters

Already a single forward simulation of a PDE model in three spatial dimensions can be demanding in terms of memory requirements and computational effort. To quantify uncertainties in the solution that are induced by random changes in model parameters, either many sample simulations are needed (like in Monte-Carlo approaches) or additional model dimensions have to be introduced (as in Galerkin-type approaches). The Galerkin-type approach of polynomial chaos expansion (PCE) bases on a (truncated) expansion of the uncertainty component in the solutions. In this PCE model, every uncertainty component adds one dimension to be discretized. It has been observed that the resulting multidimensional problem can be well approximated in a tensorized space. In this talk, we report on our recent work using Galerkin POD for tensorized bases to reduce the single dimensions optimally with respect to multidimensional snapshot data. We will introduce the relevant generalizing point of view of POD that we have successfully applied for optimal control of deterministic PDEs and show its extension to combined Finite Elements and PCE discretizations, and how it efficiently enables Uncertainty Quantification of a 3D convection-diffusion process.

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MS88

Rate-Optimal Refinement Strategies for Inference with Expensive Models

Many Bayesian inference problems involve target distributions whose density functions are computationally expensive to evaluate. Replacing the target density with a local approximation based on a small number of carefully chosen density evaluations can significantly reduce the computational expense of Markov chain Monte Carlo (MCMC) sampling. Moreover, continual refinement of the local approximation can guarantee asymptotically exact sampling. We devise a new strategy for balancing the decay rate of the bias due to the approximation with that of the MCMC variance. We prove that the error of the resulting local approximation MCMC (LA-MCMC) algorithm decays at roughly the expected $1/\sqrt{T}$ rate, and we demonstrate this rate numerically. We also introduce an algorithmic parameter that guarantees convergence given very weak tail bounds, significantly strengthening previous convergence results. We discuss generalizations of this approach, and demonstrate LA-MCMC on a computationally intensive

Bayesian inverse problem arising in groundwater hydrology.

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MS89

Can Stable and Accurate Neural Networks Be Computed? - On the Barriers of Deep Learning and Smale's 18th Problem

Deep learning (DL) has had unprecedented success and is entering scientific computing with full force. However, DL suffers from a universal phenomenon: instability, despite universal approximating properties often guaranteeing the existence of stable and accurate neural networks (NNs). We demonstrate basic well-conditioned problems in scientific computing where NNs with great approximation qualities are proven to exist, however, there does not exist any algorithm, even randomised, that can train (or compute) such a NN to even 1-digit of accuracy with a probability greater than 1/2. These results provide basic foundations for Smale's 18th problem ("What are the limits of AI?") and imply a potentially vast classification theory describing conditions under which (stable) NNs with a given accuracy can be computed by an algorithm. We begin this theory by initiating a unified theory for compressed sensing and DL, leading to sufficient conditions for the existence of algorithms that compute stable NNs in inverse problems. We introduce Fast Iterative REstarted NETworks (FIRENETs), which we prove and numerically verify (via suitable stability tests) are stable. Moreover, we prove that only $\mathcal{O}(|\log(\epsilon)|)$ layers are needed for an ϵ accurate solution to the inverse problem (exponential convergence), and that the inner dimensions in the layers do not exceed the dimension of the inverse problem. Thus, FIRENETs are computationally very efficient.

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MS89

Approximation of High-Dimensional Discontinuous Functions by Deep Neural Networks

Functions with structured singularities appear in various areas of applied math. In image processing, they are models for natural images, they appear as solutions of transport dominated PDEs, and in classification problems they model the classifiers. These functions are traditionally problematic for classical approximation methods due to their non-smoothness and often also high dimensionality. We will show that in many scenarios deep neural networks approximate high dimensional discontinuous functions with structured singularities with a similar order as if no discontinuity were present. This observation is especially striking in high dimensions, where we will demonstrate that high dimensional discontinuous functions, the singularities of which have a generalised form of bounded variation, can be approximated at a dimension-independent rate.

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MS89

A Few Thoughts on Deep Network Approximation

Deep network approximation is a powerful tool of function approximation via composition. We will present a few new thoughts on deep network approximation: given an arbitrary width and depth of neural networks, what is the optimal approximation rate of various function classes? Does the curse of dimensionality exist for generic functions? Can we obtain exponential convergence for generic functions? We will answer these questions for networks with different activation functions and discuss open questions for numerical implementation.

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MS90

Mixed Precision Randomized SVD

Randomized algorithms are a popular technique for performing low rank approximation, with many applications in scientific computing. Given a matrix A with low numerical rank, our aim is to compute cheaply some decomposition that approximates A well. Error analyses for randomized algorithms typically assume that any floating-point errors are swamped by the errors introduced by the randomization process. Focusing on the randomized SVD, we investigate how a mixed precision algorithm can be developed to balance the requirements of speed and accuracy.

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MS90

Replacing Pivoting in Distributed Gaussian Elimination with Randomized Transforms

Gaussian Elimination is the primary technique for solving dense systems of linear equations. For many problems, pivoting is necessary for numerical stability, but can add a significant overhead on distributed systems, especially when accelerated with GPUs. We discuss using recursive butterfly transforms to randomize the matrices and make pivoting is unnecessary. These transforms use an FFT-like structure, which allows them to be efficiently applied.

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MS90

Data-Aware Mixed Precision Algorithms

The accuracy of linear algebra computations is heavily dependent on the data computed with. For example, floating-point operations on numbers of small magnitude produce rounding errors of correspondingly small magnitude. This property is becoming increasingly important with the emergence of fast low precision arithmetics supported in modern hardware, and has given birth to a wide class of data-driven mixed precision algorithms, which adapt the precisions they use to the data given to them. My intention is to survey these data-driven algorithms in linear algebra, show that they share strong connections, and propose new research directions to explore within this new subfield of mixed precision HPC.

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MS90

Performance and Numerical Behaviour of Sparse Lu Factorization in Single-Precision

It is well established that mixed precision algorithms that factorize a matrix at a precision lower than the working precision can reduce the execution time and the energy consumption of parallel solvers for dense linear systems. Much less is known about the efficiency of mixed precision parallel algorithms for sparse linear systems, and existing work focuses on single-core experiments. We evaluate the benefits of using single-precision arithmetic in solving double-precision sparse linear systems using multiple cores, focusing on the key components of LU factorization and matrix-vector products. We find that single-precision sparse LU factorization is prone to a severe loss of performance due to the intrusion of subnormal numbers. We identify a mechanism that allows cascading fill-ins to generate subnormal numbers and show that automatically flushing subnormals to zero avoids the performance penalties. Our results show that the anticipated speedup of 2 over a double-precision LU factorization is obtained only for the very largest of our test problems. We also find that using single precision for the matrix-vector product kernels provides an average speedup of 1.5 over double precision kernels, but new mixed-precision algorithms are needed to exploit this benefit without losing the performance gain in the process of refining the solution to double precision accuracy.

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MS92

Contrasting Sensitivity and Data Assimilation in the Context of the Autoimmune Disease Alopecia Areata

Alopecia Areata (AA) is an autoimmune disease characterized by hair loss, often in distinct spatial patches. Hair follicles are one of the few immune privilege sites meaning foreign antigens do not elicit an immune response. The cause of AA is thought to be a catastrophic loss of immune suppression through an autoimmune guardian mechanism. We have previously developed a model that characterizes the dynamics of a both single hair follicles and larger patches of follicles, the immune guardian mechanism, and the immune system response. The model captures key characteristics of the disease and sensitivity analysis shows that there are specific processes that play a district role in the progression of the hair loss patches. Recently we began studying the inverse problem associated with taking partial observations that might be made in a clinic to estimate the disease state. Using synthetic data, we show that the data assimilation method capitalizes on sensitivity to enhance the convergence to true parameters. This is a non-intuitive result since sensitive parameters are often difficult to estimate with other methods.

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MS92

Bayesian Uncertainty Quantification for Particle-Based Simulation of Lipid Bilayer Membranes

A number of problems of interest in applied mathematics and biology involve the quantification of uncertainty in computational and real-world models. A recent approach to Bayesian uncertainty quantification using transitional Markov chain Monte Carlo (TMCMC) is extremely parallelizable and has opened the door to a variety of applications which were previously too computationally intensive to be practical. In this talk, we first explore the machinery required to understand and implement Bayesian uncertainty quantification using TMCMC. We then describe dissipative particle dynamics, a computational particle simulation method which is suitable for modeling biological structures on the subcellular level, and develop an example simulation of a lipid membrane in fluid. Finally, we apply the algorithm to a basic model of uncertainty in our lipid simulation, effectively recovering a target set of parameters (along with distributions corresponding to the uncertainty) and demonstrating the practicality of Bayesian uncertainty quantification for complex particle simulations.

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MS92

UQ and Estimation of Quantities of Interest in Safety Pharmacology Applications

The main goal of cardio-toxicity studies is to assess the impact of molecules on the electrical activity of cardiac cells. In experiments, groups of cells are monitored in a control state and when a given concentration of a molecule is injected; an electro graph is recorded (called Field Potential). The main goal is to determine, based on the recorded signals, the electrical conductivity of the different ionic channels and how they are altered by the molecule. The intrinsic variability, the heterogeneities and the parametric uncertainty of the system have to be taken into account in order to perform a robust estimation of the ionic channel properties. To this end, some methods are investigated: first, numerical strategies to account for the uncertainties of the system and build an in-silico population of experiments are presented; second, a greedy dimension reduction strategy for classification in high-dimensional setting is detailed. Several realistic test cases are presented.

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MS92

Estimating Heterogeneity in Prostate Cancer and its Effect on Treatment Resistance

Prostate cancer is treated with hormonal therapy, which is very successful initially but eventually becomes resistant. Without accounting for the phenotypic heterogeneity present in tumors, it is impossible to reliably predict treatment outcomes or the onset of treatment resistance. While mathematical models have been developed to incorporate structured heterogeneity, little work has been done to validate and parameterize these models with aggregate preclinical or clinical data. It is difficult to ascertain cellular heterogeneity from clinical data such as biomarker measurements, since clinical data is aggregated and does not provide information about the various subpopulations of the tumor (e.g., how sensitive or resistant they are to treatment). Here we discuss a mathematical methodology to discover the underlying distribution of sensitive and resistant tumor cells using aggregated clinical data from prostate cancer patients. These distributions are then used to predict the likelihood of success of additional treatment cycles.

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MS93

A Process-Based Forecast of Near-Term Distributional Shifts in Marine Species

Species around the globe are shifting their geographical ranges in response to climate change. Accurate, near-term prediction of their future distributions is critical for natural resource management and biodiversity conservation. At short time scales, transient dynamics of populations not in equilibrium with the environment may strongly influence species distributions, underscoring the need to explicitly model demography. We developed a process-based dynamic range model that estimates demographic rates, and the relationship between those rates and the environment, to forecast species range shifts in response to temperature change. This hierarchical Bayesian model uses only data on species occurrences and abundances to estimate parameters and simulate future states. We fitted this model to historical occurrence and abundance data from demersal trawl surveys conducted annually by the National Oceanic and Atmospheric Administration since the 1960s. We focused on four species of importance to fisheries in the mid-Atlantic region summer flounder, shortfin squid, spiny dogfish, and gray triggerfish and made forecasts for every year up to a decade (2009-2018). We then compared our annual forecasts to the real data from the testing interval, and to predictions from correlative models. The dynamic range model outperformed a generalized additive model in explaining historical species distributions when tested on out-of-sample data. Incorporating stage-structured population dynamics improved forecast skill. Ongoing work will expand on model evaluation and comparison, and address the selection of appropriate observation models. This work is among the first applications to real data of a class of models that shows great promise in ecological forecasting: dynamic range models that can make mechanistic predictions about the future by estimating process rates from survey data. By explicitly modeling demographic processes, this study advances the ability to predict short-term range dynamics of species on the move.

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MS93

Modeling Optimal Responses in a Changing Arctic

Animals must balance a series of tradeoffs in order to maximize their fitness, continuously balancing risks and rewards. Their decisions depend on complex interactions between environmental conditions, behavioral plasticity, reproductive biology, and energetic demands. As animals respond to novel environmental conditions caused by climate change, their optimal decisions may shift. Stochastic dynamic programminga stochastic optimal control approachprovides a flexible modeling framework within which to explore these trade-offs, but this method has not yet been used to study possible changes in optimal behaviors caused by climate change. We created a stochastic dynamic programming model capturing trade-off decisions required by an individual adult female polar bear as well as the fitness consequences of her decisions. We predicted optimal foraging habitat selection throughout her lifetime as well as the energetic thresholds below which it is optimal for her to abandon a reproductive attempt. To explore the effects of climate change, we shortened the spring feeding period by up to 3 weeks, which led to predictions of shifted foraging habitat use and higher reproductive thresholds. The resulting changes in fitness may be interpreted as a best-case scenario, where bears adapt instantaneously and optimally to new environmental conditions.

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MS93

Soil-Climate Feedbacks: Illuminating Black Box Simulations with Math

Soil carbon stocks have the potential to be a strong source or sink for carbon dioxide over the next century, playing a critical role in climate change. Yet there was little agreement on soil carbon stocks between 11 Earth system models (ESMs) in the Climate Model Intercomparison Project 5. Predicted present-day stocks ranged from roughly 500 Pg to over 3000 Pg and predicted changes over the 21st century ranged from -70 Pg to +250 Pg. Why do such large differences exist between the models and are they all right? Examining the codebase for all ESMs was intractable. Instead, we fit a simplified model to ESM simulation outputs based on underlaying documented mathematical structure and initialization routines. We were able to explain most of the underlaying simulation behavior using this reduced complexity model. In general, model differences were explained by different in parameterization and inputs (mass and temperature), not underlaying structure. Furthermore, this variation reflects real world uncertainties in our observations, implying that the soil carbon response to climate change is extremely uncertain over the next century.

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MS93

Modeling the Growth, Spread, and Control of the Invasive Eurasian Watermilfoil

Eurasian watermilfoil (EWM) is one of the most invasive aquatic plants in the US, found throughout most of the US and in Southern Canada and introduced into North America in the 1940s (originating from Europe, Asia, and North Africa). Like other invasive plants, EWM has the ability to grow and spread quickly, forming dense monocultures, due to its ability to outcompete many native aquatic plants. Expanding on previous theoretical models, we use an ordinary differential equation (ODE) approach to model the growth of IWM, which depends on lake characteristics such as lake clarity, available nutrients, temperature, and depth, and a partial differential equation (PDE) model to account for seasonal diffusion of the plants roots (stolons). In addition, we describe some of the field work being done on the infested Lake Norwood in Upstate NY, where EWM samples are being taken to fit modeling results. One of the main parts of this project is to design a sustainable approach, to aid in EWM reduction with minimal cost and effort by influenced lake stakeholders. With this in mind, we show using numerical simulations how various control techniques, such as localized handpulling and placement of mats that block sunlight, can be used to mitigate EWM invasions. In addition, another appealing control technique is the use of biocontrol to reduce EWM. Here, we describe a machine-learning approach that predicts biocontrol success (the milfoil weevil)) at EWM reduction. To develop our predictive model, we first performed a metadata analysis from 133 published peer-reviewed literature and professional reports of weevil augmentation field experiments, collecting data lake characteristics (limnological and landscape) and weevil augmentation strategies. The predictive model works by learning patterns among lake characteristics, along with the recorded augmentation strategy (absolute number of weevils, number of applications) and the reported success of each study.

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MS94

Selectivity of the KcsA Potassium Channel: Analysis and Computation

Ion channels regulate the flux of ions through cell membranes and play significant roles in many physiological functions. Most of the existing literature focuses on computational approaches based on molecular dynamics simulation or numerical solution of the modified Poisson-Nernst-Planck (PNP) system. In this paper, we present an analytical and computational study of a mathematical model of the KcsA potassium channel, including the effects of ion size (Bikerman model) and solvation energy (Born model). Under equilibrium conditions, we obtain an analytical solution of our modified PNP system, which is used to explain selectivity of KcsA of various ions. For the nonequilibrium cases, due to difficulties associated with a pure analytical or numerical approach, we use a hybrid analytical-numerical method to solve the modified PNP system. Our predictions of selectivity of KcsA channels and saturation phenomenon of the current-voltage (I-V) curve agree with experimental observations.

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MS95

Numerical Evidence for the Validity of the Kinetic Wave Equation

In this talk, I will present joint work with Banks, Korotkevich, Kovacic and Shatah related to the validity of kinetic wave equation (KWE) for the Nonlinear Schrdinger equation under certain scaling regimes. More specifically, I will provide numerical evidence that supports the validity of the KWE under regimes predicted by theory. I will link this work to prior analytical work of myself, Germain, Hani and Shatah.

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MS95

Description of Potential Fluid Flow with Free Surface by Singularities of Analytic Functions

As evident from numerical simulations of free surface waves in conformal variables, the fluid flow can be described by analytic functions with square–root type branch points. We introduce a complex fluid potential having exactly two square–root branch points, and formulate a system of pseudo-differential PDEs posed on a branch cut connecting these points. This result is of fundamental importance for understanding of formation of singularities on the free surface of ideal fluid in 2D. The present approach allows generalization two multiple pairs of branch points. Pairs of branch points may be viewed as particles with long range interactions.

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MS95

Is Dark Matter a Manifestation of Energy Trapped in Pattern Structures?

We investigate the origin of the flattening of the rotation curves for both HSB and LSB disk galaxies and many of the observed scaling relations from the point of view that 'dark matter' may simply be a manifestation of energy trapped in pattern defects arising as the result of gravitationally induced instabilities of ordinary baryonic matter. Our theory leads to detailed rotation curves, to the Tully-Fisher (BFTR), the radial acceleration relation (RAR), the Freeman Law and provides a physical mechanism to explain the effectiveness of MOND theory.

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MS95

On the Derivation of the Kinetic Wave Equation

Wave turbulence is out-of-equilibrium statistical mechanics of random weakly nonlinear dispersive waves. It conjectures the existence of a kinetic wave equation which describes the evolution of the expected value of the square of the amplitude of the Fourier modes. This description is supposed to occur at a time scale depending on wavelength localization and the strength of the nonlinearity. In this talk we will describe theoretical and numerical results towards confirming this conjecture.

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MS96

Variational Characterization of Order Parameters in Stochastic Dynamical Systems

A prevalent theme in quantitative science is the prediction of emergent large-scale phenomena in systems consisting of many microscopically interacting entities. Examples include molecular dynamics, traffic flow and sociodynamics. The identification of representative macroscopic observables (also known as order parameters or reaction coordinates, depending on context), often marks the first step for understanding these phenomena. In the first half of my talk, I will present how the problem of identifying optimally-consistent order parameters from microscopic simulation data can be posed as a variational prob-

lem that is accessible to modern machine learning methods, such as deep neural networks. Such methods are however notorious for demanding a large amount of training data in order to develop their full predictive capacity. In the case of predicting order parameters, one might expect that the amount of simulation data needs to grow with the size of the system, and in the worst case depends exponentially on the dimension of the state space. I will show that under the right re-formulation of the variational problem this is not the case, and that the data requirement depends only on the dimension of the optimal order parameter.

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MS96

Exploring High Dimensional Configuration Spaces of Molecules using Reinforced Dynamics

Enhanced sampling methods such as metadynamics and umbrella sampling have become essential tools for exploring the configuration space of molecules and materials. At the same time, they have long faced the following dilemma: Since they are only effective with a small number of collective variables (CVs), choosing the right CVs become critical for their accuracy. Yet until now, we still lack systematic methodologies for selecting the correct CVs. In this talk, we will demonstrate that reinforced dynamics can be used to efficiently explore the configuration space and free energy landscapes with a large set of CVs, thereby alleviating the difficulty associated with choosing the right CVs. We illustrate this by studying various representative and challenging examples.

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MS96

Automatic Differentiation to Simultaneously Identify Nonlinear Dynamics and Extract Noise Probability Distributions from Data

The sparse identification of nonlinear dynamics (SINDy) is a regression framework for the discovery of parsimonious dynamic models and governing equations from time-series data. As with all system identification methods, noisy measurements compromise the accuracy and robustness of the model discovery procedure. In this work, we develop a variant of the SINDy algorithm that integrates automatic differentiation and recent time-stepping constrained motivated by Rudy et al. for simultaneously (i) denoising the data, (ii) learning and parametrizing the noise probability distribution, and (iii) identifying the underlying parsimonious dynamical system responsible for generating the time-series data. Thus within an integrated optimization framework, noise can be separated from signal, resulting in an architecture that is approximately twice as robust to noise as state-of-the-art methods, handling as much as 40% noise on a given time-series signal and explicitly parametrizing the noise probability distribution. We demonstrate this approach on several numerical examples, from Lotka-Volterra models to the spatio-temporal Lorenz 96 model. Further, we show the method can identify a diversity of probability distributions including Gaussian, uniform, Gamma, and Rayleigh.

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MS96

Identification of Information Bottleneck for Model Reduction of Stochastic Systems

Model reduction is one of the most important problems for analysis of complex physical and chemical processes in many scientific disciplines. The general aim of model reduction is to find a small number of observations of the system state, usually called reaction coordinate (RC), and project the original kinetics to the space of the observations so that the essential part of the full kinetics can be accurately characterized. The information bottleneck provides a powerful analysis tool for the model reduction of stochastic systems, but the identification algorithm of information bottleneck remains challenging for nonlinear and high-dimensional stochastic systems. In this talk, we will introduce some novel deep learning based algorithms for this problem. In contrast with existing algorithms, our algorithms can (i) provide the explicit representation of the full-state kinetics reconstructed from the reduced model, and (ii) lead to an interpretable reduced kinetic model due to the practical requirements.

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MS97

Dynamic Behavior of Fluid-Conveying Pipe under Axial Force and Travelling Load

In this study, the problem of the dynamic behaviour of fluid-conveying pipe under axial force and travelling load is considered. The Generalized Galerkin Method (GGM) is used to reduce the governing fifth order partial differential equation(PDE) to a set of ordinary second order differential equation(ODE). Impulse response function is further used to treat this problem to obtain analytical solution.Analytical solution of this problem is obtained and various results depicting the effects of vital parameters of the system on the vibration of the fluid-conveying pipe are presented. Vibration profiles of the vibrating system are presented for various values of Fluid Velocity, Axial Tension, Natural frequency, the Damping parameter and Foundation Stiffness. Faculty Advisors: Babatope Omolofe, Federal University of Technology Akure, bomolofe@futa.edu.ng

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MS97

Accelerated Alternating Minimization for X-ray

Tomographic Reconstruction

While Computerized Tomography (CT) images can help detect disease such as Covid-19, regular CT machines are large and expensive. Cheaper and more portable machines suffer from errors in geometry acquisition that downgrades CT image quality. The errors in geometry can be represented with parameters in the mathematical model for image reconstruction. To obtain a good image, we formulate a nonlinear least squares problem that simultaneously reconstructs the image and corrects for errors in the geometry parameters. We develop an accelerated alternating minimization scheme to reconstruct the image and geometry parameters. Faculty Advisors: Nagy, James, Emory University, jnagy@emory.edu

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MS97

Analyzing Gyrostat Equilibria using Numerical Algebraic Geometry

A gyrostat, first designed by Lord Kelvin, is a gyroscope encased in a rigid box. Its dynamical properties are controlled by six homogeneous representing inertia and angular momentum of the wheel with the steady-state solutions of the gyrostat are dependent on the parameters. This talk will discuss an analysis of the parameter space of a simplified gyrostat model with only three homogeneous parameters using numerical algebraic geometry in spherical coordinates to compute the connected components of the parameter space with the same steady-state solution behavior. This is joint work with Jonathan Hauenstein. Faculty Advisors: Jonathan Hauenstein, Professor at the University of Notre Dame, hauenstein@nd.edu

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MS97

Density of States Graph Kernels

A fundamental problem on graph-structured data is that of quantifying similarity between graphs. Graph kernels are an established technique for such tasks; in particular, those based on random walks and return probabilities have proven to be effective in wide-ranging applications, from bioinformatics to social networks to computer vision. However, random walk kernels generally suffer from slowness and tottering, an effect which causes walks to overemphasize local graph topology, undercutting the importance of global structure. To correct for these issues, we recast return probability graph kernels under the more general framework of density of states — a framework which uses the lens of spectral analysis to uncover graph motifs and properties hidden within the interior of the spectrum — and use our interpretation to construct scalable, composite density of states based graph kernels which balance local and global information, leading to higher classification accuracies on benchmark datasets. Faculty Advisors: Bindel, David, Cornell University, Bindel@cs.cornell.edu

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MS97

Predicting Time-Delayed Chaotic Dynamical Systems with Machine Learning

The dynamics of physiological systems are significantly impacted by delay. The time-delay caused by the transport and processing of chemical components and signals may be of significant consequence. Biological systems present a challenge to model, analyze and predict. The utilization of machine learning to build mathematical models of complex systems has rapidly grown. For time-dependent series, generally a recurrent neural network (RNN), capable of returning past states, is used. In most common RNN implementations, multiple hidden layers are rebalanced during training to achieve adequate results. However, these implementations can be computationally expensive and may require extensive training data. Here, we utilize a type of RNN called an echo state network (ESN), a static, randomly initialized reservoir of nodes. We study systems exhibiting chaotic time-delay such as the degrade-and-fire circuits and delay-linear shear flow, with a primary focus on the physiological insulin-glucose system. Manipulating only signal propagation and input smoothing, we model these systems with generated reservoirs. In future works, we will further tune the reservoir, addressing stability and noise. We intend to research the use of other machine learning techniques in determining the optimal parameters for reservoir generation. Faculty Advisors: Ott, William, University of Houston, wrott@central.uh.ed

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MS97

Anderson Localization of Walking Droplets in a Random Topography

In this talk, we describe the first classical model for Anderson localization of conduction electrons by demonstrating analogous localization phenomena in a hydrodynamic pilot-wave system. Anderson localization is understood exclusively as a wave interference effect; we are taught that no deterministic particle-based theory can rationalize the localization of electrons in disordered media. We are thus forced to neglect the twofold nature of quantum systems as both particles and waves. By examining the emergent statistics of a wave-driven walking droplet as a classical analog of a quantum particle guided by the Schrdinger equation, we demonstrate that Anderson localization can be rationalized by a deterministic pilot-wave interpretation of quantum mechanics, such as the de Broglie-Bohm theory. As the first particle-based model for Anderson localization, our project contributes to the rapidly growing list of quantum phenomena reproduced with pilot-wave hydrodynamics, motivating the use of such model systems for classical and mechanistic interpretations of the counter-intuitive predictions made by quantum mechanics. Faculty Advisors: Pedro Saenz, Physical Mathematics Laboratory, saenz@unc.edu

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MS97

Numerical Experiments in compuGUT

The colon is a difficult area to research and perform experiments on due to its physical inaccessibility within the body. We run numerical experiments in a software package called compuGUT, that is used to simulate intestinal digestion and fermentation as fiber moves through the colon. This program was created with the intention of being accessible to scientists even if they had limited programming knowledge through the use of user-friendly adjustment of parameters. The process of digestion, exchange, and transport that occurs within the colon is described by a set of mathematical models. Due to the complexity of the models, computational methods were implemented to approximate this solution. In order to determine the sensitivity of the approximate solution, we perturb parameters by small numerical values. Then by comparing the perturbed solution to the original solution, we can gain insight into the sensitivity of the solution with respect to each parameter. This presentation will give a general overview of how compuGUT works and some preliminary results. Faculty Advisors: Melara, Luis, Advisor, lamelara@ship.edu

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MS97

Exploring the Ability of Reservoir Computers to Learn Chaotic Systems

A Reservoir Computer is a machine learning model governed by an ordinary differential equation with an internal complex network. We experimented with millions of Reservoir Computers that were applied to learn and predict the chaotic dynamics described by the Lorenz Attractor. We examined the dynamics and numerical findings of these experiments. We investigated how predictability is affected by different topologies of the internal network including extremely sparse versions of these networks. Another hyper-parameter in the experiments was the spectral radius of the internal network as controlled by a rescaling of the adjacency matrix to yield the desired spectral radius. Numerous experiments describe an interesting interaction between these two hyper-parameters, namely the sparsity and spectral radius of the network. When models have no edges removed then they perform well with a small spectral radius. Remarkably, when edge removal is increased to 70% or above, then a higher spectral radius will yield better predictors of Chaos than standard models. These experiments suggest that the spectral radius hyper-parameter and the random edge removal percentage of the network combine in unexpected ways to improve predictability. These experiments illustrate design principles to enhance learning of Reservoir Computers on Chaotic Systems like the Lorenz Attractor. Faculty Advisors: Webb, Benjamin, Brigham Young University,bwebb@math.byu.edu

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MS98

Regularized Stokeslets for Geometric Effects on Locomotion

Helicobacter pylori is a bacterium which infects the human stomach, where it is known to cause ulcers and stomach cancer. It has a helical cell body and swims using rotating flagellar filaments. First, combining imaging of swimming *H. pylori* and numerical modeling using the method of Regularized Stokeslets, we investigate how much advantage the helical shape can provide for swimming through Newtonian fluids. We find that it only increases swimming speed by at most 15% relative to rod-shaped cells. Second, while swimming through the gastric mucus on its way to colonize the epithelium, *H. pylori* actively remodels its surrounding by generating ammonia that turns the nearby gel into a fluid pocket. We investigate how this active remodeling produces complex three-dimensional confinement of the swimming bacteria, and show how three-dimensional confinement affects swimming in different ways than two-dimensional confinement. Both the bacterium and the confinement by nearby gel are modeled using the method of Regularized Stokeslets.

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MS98

Cell-Body Rocking and the Synchronization of Flagella

Flagella and cilia are widespread across eukaryotic cells and their coordinated beating is integral to many important biological processes. The origin of this synchronization is an active area of research. In this talk, a previously proposed integrative 2d model of the structure and internal force generating mechanisms of a flagellum is extended to three dimensions. The resulting fluid-structure interaction is modeled using the method of regularized Stokeslets combined with a system of images that allows the no-slip condition to be enforced on spherical surfaces. This model is used to investigate the influence cell-body rocking has on the hydrodynamical coupling between flagella.

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MS98

Force and Torque Free Swimming near a Boundary

The hydrodynamic effects of a nearby boundary are likely to be important in the evolution of bacterial motility. We use the method of images for regularized Stokeslets in numerical simulations to investigate these effects by modeling bacteria of different body sizes and helical geometries swimming near a wall. We verify the results from the numerical simulations with scaled macroscopic experiments using rotating cylinders, translating cylinders and constrained rotating helices of different wavelengths. We compare our numerical and experimental results for rotating cylinders to the theory by Jeffrey and Onishi. Their theory is confirmed by our results and it provides a benchmark for establishing the correct blob size of regularized Stokeslets in numerical simulations on a cell body. The blob size on the helical flagellum is chosen to match the numerical results with the experimental ones. We also find that the propulsive efficiency of bacterial swimming increases for all helical wavelengths when our model is near a wall, and that the maximum increase in efficiency occurs for biologically relevant helical wavelengths. Our results show that the body sizes of bacteria are also close to this optimum for maximal swimming speed. These results suggest that boundary effects exert an important selective pressure on bacterial evolution because biological values are close to the optimal flagellum wavelength and optimal body size necessary for efficient swimming near a boundary.

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MS98

Collective Swimming and Its Implications for Reproduction

Undulatory filaments are vital for many cellular- and organism-level processes. These filaments typically serve to move fluid as well as propel cells, depending on the context. In this talk, we focus on the collective motion of filaments in a Stokesian fluid, where regularized Stokeslets are used to model forces exerted along the filament. Our model is based on the dynamics of sperm, who swim in highly heterogeneous, viscous fluid environments, and exhibit collective behavior in some species. We will explore the energetic implications of collective swimming, both in free-space and near surfaces, and relate this to reproductive strategies.

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MS99

Data-Driven Modeling of Subgrid-Scale Processes using Deep Neural Nets and Transfer Learning

Resolving all the relevant length and time scales in many fluid flow simulations, particularly of turbulent flows, is computationally challenging. In practice, low-resolution models resolve the large-scale processes while the effects of the small-scale processes are often parameterized in terms of the large-scale variables. In the past few years, non-parametric data-driven parameterization (DD-P) using deep learning has shown promising results, but numerical stability (in online or a posteriori simulations) and generalization (i.e., extrapolation) have remained as challenging and important issues to address. In this talk, using 1D forced Burgers and 2D turbulent flows as testbeds, we 1) show the promises of DD-P, once correctly trained, in representing subgrid-scale effects, in particular by capturing energy backscattering, while remaining numerically stable, and 2) demonstrate how transfer learning enables DD-P to generalize to flows with higher Reynolds numbers and different numerical resolutions.

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MS100

Calculating the 3D Kings Multiplicity Constant

We present lower and upper bounds for $F(k_1, k_2, k_3)$, the number of configurations of non-attacking kings on a 3-D chess board of dimensions $k_1 \times k_2 \times k_3$. We develop techniques to compress adjacency matrices enabling us to compute eigenvalues of matrices with dimensions up to 157M by 157M. We obtain

$$1.1722475193 \leq \lim_{k_1,k_2,k_3\to\infty} F(k_1, k_2, k_3)^{1/k_1k_2k_3} \leq 1.179842897.$$

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MS100

Recent Progress in the Rational Factorisation of Integer Matrices

We identify and analyse obstructions to factorisation of integer matrices into products N^TN or N^2 of matrices with rational or integer entries. The obstructions arise as quadratic forms with integer coefficients and raise the question of the discrete range of such forms. They are obtained by considering matrix decompositions over a superalgebra in which we identify a co-Latin symmetry space.

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MS100

Bohemian Inners Inverses: A First Step Toward Bohemian Generalized Inverses

Inner inverses are a particular type of generalized inverses. More precesily, for a given m x n matriz A, over a field K, the n x m matrices X, over K, satisfying that AXA = A, are called inner inverses of A. Inner inverses, due to Urquhart Theorem, play an important role in the representation of many other generalized inverses, and have the geometric property of being an affine linear space. In this talk we will study the inner inverses, being bohemian, of a bohemian matrix, all over the same population. In particular we will be dealing with some particular families of bohemians and, for them, we will show a complete description of the corresponding bohemian inners. In addition, when the population is restricted to 0, 1, -1, we will show exact formulas for the cardinality of the set of all bohemian inner matrices of a given bohemian matrix. The work in this talk has been partially supported by the Spanish Ministerio de Economia y Competitividad, and by the European Regional Development Fund (ERDF), under the Project MTM2017-88796-P.

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MS100

Which Columns are Independent? Why does Row Rank = Column Rank?

At the start of a linear algebra course, we want to recognize independent columns without using elimination. Small Bohemian matrices A are great candidates. If columns 1 and 2 are independent then they go into C. Suppose column 3 of A equals column 1 + 5 (column 2). The goal is to see how matrix multiplication A = CR needs 1,0 and 0,1 and 1,5 in the columns of R. Here is a special but important case. Suppose every column of A is a multiple of column 1. Then all rows are multiples of one row. This starts with experiment and grows into proof. Gradually the great fact emerges that column rank equals row rank. The course is on its way.

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MS101

Fast and Efficient Multi-Domain Learning, A Software and Hardware Co-Design Perspective

Nowadays, one practical limitation of deep neural network (DNN) is its high degree of specialization to a single task or domain (e.g. one visual domain). It motivates researchers to develop algorithms that can adapt DNN model to multiple domains sequentially, meanwhile still performing well on the past domains. This process of gradually adapting DNN model to learn from different domain inputs over time is known as multi-domain learning. In this talk, we will present his recent research in developing fast and efficient multi-domain learning method from a software and hardware co-design perspective.

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MS102

Reduced Order Modeling and Deep Learning of Turbulent Reacting Flows

Some of the principal impediments of high-fidelity simulation of turbulent hydrocarbon flames are: (i) Keeping track of O(1000) number of species, each requiring solution of a transport partial differential equation (PDE). (ii) Modeling of the effects of turbulence, particularly turbulence-chemistry interactions. (iii) Solving high dimensional equations describing turbulent combustion closures, such as those in transported probability density function (PDF) methods. In this work, we present an arsenal of techniques from deep learning to reduced order modeling to tackle these open problems in reactive turbulence simulations. We present a novel on-the-fly reduced order modeling methodology to significantly reduce the computational cost of solving the species transport equation by exploiting correlations between species. We present a physics-informed neural network for learning the unclosed terms in the PDF transport equation from high fidelity numerical or experimental data. We also present a novel approach for solving high-dimensional PDF transport equation using time-dependent basis. We demonstrate that this method overcomes the curse of dimensionality and does not have the limitations of Monte-Carlo based Lagrangian PDF solvers.

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MS102

Structure-Infused Autoencoders for Generative and Reduced Order Modeling of Spatio-Temporal Dynamics

This works describes the design of variational autoencoders for generative modeling and and reduced order modeling of spatio-temporal dynamics. Particular emphasis is on the choice of priors and constraints to ensure that the latent manifold is interpretable and robust enough to be learnt with small amounts of data. Priors are enforced via a hierarchical Bayesian approach which is implemented as a nested variational autoencoder within the variational autoencoder. The geometry of the latent space is shaped via the use of Riemannian metrics. Applications are demonstrated on model combustion problems with an emphasis on predictions in regions of sparse data.

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MS102

Construction of Non-Equilibrium Hydrodynamic Models: Combining Physics and Machine Learning

The talk presents a new paradigm for the construction of predictive modeling for the description of non-equilibrium hypersonic flows from a fundamental physics perspective, rejecting the empiricism that has prevented progress in the modeling of hypersonic flows for decades. This effort will establish the first physics-aware reduced-order model which relies on a robust Coarse-Grain modeling technique enhanced by physics-infused adaptive neural networks. The methodology can significantly improve the accuracy, robustness, and computational efficiency of physical models for complex multi-physics hypersonic flows. Substantial progress in the area of computational mathematics and machine learning have allowed to carry out tasks that a decade ago seemed unachievable. Particularly interesting are the Physics-Informed Reduced Order Models, which allow for integration of physical constraints into the reduced order models. We will cover the key aspects involved in model development, namely: (1) using ab-initio quantum calculations as a powerful tool to construct high-fidelity physics-based models; (2) defining reduced-order models for the simulation of 3D flows leveraging a Maximum Entropybased coarse grain model and deep learning to solving partial differential equations, to enhance computational complexity while ensuring compliance with physics; (3) validating physical models leveraging the most recent developments in Uncertainty Quantification algorithms.

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MS102

Global Convergence of PDE Models with Neural Networks

We rigorously study the optimization of a class of partial differential equations (PDEs) with neural networks, specifically linear elliptic PDEs with neural network source terms. The neural network parameters in the PDE are optimized using gradient descent where the gradient is evaluated using an adjoint PDE. As the number of parameters become large, the PDE and adjoint PDE converge to a non-local PDE system. Using this limit PDE system, we are able to prove convergence of the neural network-PDE to a global minimum during the optimization. The limit PDE system contains a non-local linear operator whose eigenvalues are positive but become arbitrarily small. The lack of a positive lower bound (i.e., a spectral gap) on the eigenvalues poses the main challenge for the global convergence proof. Careful analysis of the spectral decomposition of the coupled PDE and adjoint PDE system is required.

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MS103

Nonlinear Eigenvalue Problems in the Theory of Lattice Waves

Traveling waves in Hamiltonian lattices can often be interpreted as eigenfunctions of certain nonlinear integral operators. We discuss how this setting can be used to prove the existence of waves, to implement efficient numerical schemes, and to derive simplified formulas for asymptotic regimes. We further address the notoriously difficult uniqueness problem and present first results for a simple toy model.

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MS103

Language Growth and Death on a Square Lattice

We consider a language dynamics ODE model for two languages on a square lattice which is an extension of the one popularized by Abrams and Strogatz. The coupling between adjacent sites is inherently nonlinear. For this model we are interested in the existence and spectral stability of structures such as stripes and spots, and the dynamics associated with perturbations of these structures. The competition between the inter-site coupling strength and the prestige of the language has interesting dynamical consequences. In particular, the competition leads to conditions which allow for a language to spread through the network, or alternatively die. This is joint work with Panayotis Kevrekidis.

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MS103

Non-Reciprocal Lattices with Wave Redirection Features: Theory and Experiment

We study the non-reciprocal acoustics of a disordered 2D network of two nonlinear dissipative lattices with weak linear inter-lattice coupling. Each lattice consists of linearly grounded unit cells coupled by essentially nonlinear intralattice stiffnesses. This system enables irreversible passive wave redirection from an impulsively excited lattice to an absorbing one, governed by the spatial macroscopic analogue of the Landau-Zener tunneling (LZT) quantum effect. We theoretically show that LZT wave redirection occurs only for appropriate selection of the lattice parameters and predict it to be robust over a definite energy range. Wave redirection is in the form of propagating breathers and is passively tunable (self-adaptive) to the impulse intensity (energy). The predictions are validated by experiments by means of a lattice fixture which was built according to theoretical predictions, and the different regimes of the nonlinear acoustics are experimentally recovered. In addition, we experimentally confirm the nonreciprocal acoustics of the experimental lattice system, in good agreement with theory. Our results prove the efficacy of passive wave redirection in practical dissipative lattice systems combining nonlinearity, weak coupling and asymmetry.

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MS103

Random FPUT Chains

We consider a linear Fermi-Pasta-Ulam-Tsingou lattice with random spatially varying material coefficients. Using the methods of stochastic homogenization we show that solutions with long wave initial data converge in an appropriate sense to solutions of a wave equation. The convergence is both strong and almost sure, but the rate is quite slow. The technique combines energy estimates with powerful classical results about random walks, specifically the law of the iterated logarithm.

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MS104

A Posteriori Error Analysis for a Space-Time Parallel Algorithm: Parareal in Time and Domain Decomposition in Space

This talk presents error estimates for the numerically computed value of a quantity-of-interest (QoI) when time-parallel and spatial domain decomposition techniques are employed for the approximation of the solution of a parabolic partial differential equation (PDE). In particular, we consider two algorithms: the Parareal algorithm and a Parareal-Domain Decomposition Algorithm. The Parareal algorithm is a time-parallel method to solve PDEs while, as the name suggests, the Parareal-Domain Decomposition algorithm also employs a parallel domain decomposition strategy in space in addition to the time-parallelism of the Parareal method. The error estimates developed in this work decompose the error in the QoI due to spatial and temporal discretizations, as well as quantifying the effect of Parareal and domain decomposition iterations.

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MS104

High-Order Local Propagation Algorithms for Hyperbolic Problems

Local domain-of-dependence is a fundamental feature of hyperbolic pdes. Mathematically, this means that updates of the solution at a point or in an element over a time step can be expressed as the action of some integral operator applied to neighboring data. In ideal circumstances this fact enables the use of standard explicit time stepping methods with time step constrained only by the CFL restriction. However, in the presence of local refinements or even due to the use of artificially stiff differentiation operators, the standard methods require small steps. In this talk we describe techniques which are both explicit and do not affect the global time steps.

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MS104

Fast Parallel Solution of Fully Implicit Runge-Kutta Methods for Numerical PDEs

Fully implicit Runge-Kutta (IRK) methods have many desirable accuracy and stability properties as time integration schemes, but are rarely used in practice with large-scale numerical PDEs because of the difficulty of solving the stage equations. Here we introduce a theoretical and algorithmic framework for the fast, parallel solution of the (non)linear equations that arise from IRK methods applied to (non)linear numerical PDEs, including PDEs with algebraic constraints. The new method is built using the same preconditioners needed for backward Euler-type time stepping schemes. Several new linearizations of the nonlinear IRK equations are developed, offering faster and more robust convergence than the often-considered simplified Newton. Inverting these linearizations requires solving a set of block 1×1 or 2×2 systems. Under quite general assumptions on the spatial discretization, it is proven that the preconditioned operator has a condition number of $\sim \mathcal{O}(1)$, with only weak dependence on the number of stages. The new methods are applied to several challenging fluid flow problems, including the compressible Euler and Navier Stokes equations, and the vorticity-streamfunction formulation of the incompressible Euler and Navier Stokes equations.

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MS104

High-Order Parallel in Time Multiderivative IMEX

Solvers

In this work, we present a novel class of parallelizable high-order time integration schemes for the approximate solution of additive differential equations. The methods achieve high order through a combination of a suitable quadrature formula involving multiple derivatives of the right-hand side of the differential equation and a predictor-corrector ansatz. The latter approach is designed in such a way that parallelism in time is made possible. We present thorough analysis as well as numerical results that showcase scaling opportunities of methods from this class of solvers.

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MS105

Optimal Experimental Design for Variational System Identification of Material Physics Phenomena

We focus on the problem of identifying underlying governing PDEs—i.e. system identification—for the evolution of patterns or microstructures in materials. We first employ a variational approach taking advantage of the weak form finite-element formulation, thus allowing the incorporation of boundary conditions, and ultimately leading to a linear regression problem. While the effectiveness of this method has been previously demonstrated with synthetic data that is rich in both space and time, real-life laboratory specimen will only be sparsely available due to the expensive and time-consuming nature of these experiments. Therefore, it is important to carefully design when and where to best acquire these experimental measurements. We describe an optimal experimental design procedure to select the best sampling times, targeting to minimize the estimator covariance of the PDE coefficients through expected linear A- and D-optimal design criteria. We demonstrate this method on a materials physics problem, starting with the identification among Allen-Cahn, Cahn-Hilliard, and diffusion-reaction PDEs.

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MS105

PhyCRNet: Physics-Informed Convolutional-Recurrent Network for Solving Spatiotemporal PDEs

Partial differential equations (PDEs) play a fundamental role in modeling and simulating problems across a wide range of disciplines. Recent advances in deep learning have shown the great potential of physics-informed neural networks (PINNs) to solve PDEs as a basis for data-driven modeling and inverse analysis. However, the majority of existing PINN methods, based on fully-connected NNs, pose intrinsic limitations to low-dimensional spatiotemporal parameterizations. Moreover, since the initial/boundary conditions (I/BCs) are softly imposed via penalty, the solution quality heavily relies on hyper-parameter tuning. To this end, we propose a novel physics-informed convolutional-recurrent learning architecture (PhyCRNet) for solving PDEs without any labeled data. Specifically, an encoder-decoder convolutional long short-term memory network is proposed for low-dimensional spatial feature extraction and temporal evolution learning. The loss function is defined as the aggregated discretized PDE residuals, while the I/BCs are hardly encoded in the network to ensure forcible satisfaction (e.g. periodic boundary padding). The performance of PhyCRNet has been assessed by solving three nonlinear PDEs, and compared against the start-of-the-art PINN. The numerical results demonstrate the superiority of PhyCRNet in solution accuracy and extrapolability/generalizability.

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MS105

Learning Stochastic Closures Using Sparsity-Promoting Ensemble Kalman Inversion

Closure models are widely used in simulating complex systems such as turbulence and Earths climate, for which direct numerical simulation is too expensive. Although it is almost impossible to perfectly reproduce the true system with closure models, it is often sufficient to correctly reproduce time-averaged statistics. Here we present a sparsity-promoting, derivative-free optimization method to estimate model error from time-averaged statistics. Specifically, we show how sparsity can be imposed as a constraint in ensemble Kalman inversion (EKI), resulting in an iterative quadratic programming problem. We illustrate how this approach can be used to quantify model error in the closures of dynamical systems. In addition, we demonstrate the merit of introducing stochastic processes to quantify model error for certain systems. We also present the potential of replacing existing closures with purely data-driven closures using the proposed methodology. The results show that the proposed methodology provides a systematic approach to estimate model error in closures of dynamical systems.

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MS106

Lamellar: PGAS + Active Messaging in Rust

Lamellar (https://github.com/pnnl/lamellar) is an investigation of the applicability of the Rust systems programming language for HPC as an alternative to C and C++, with a focus on PGAS approaches. Lamellar provides several different communication patterns to distributed applications. First, Lamellar allows for sending and executing active messages on remote nodes in a distributed environments. The runtime supports two forms of active messages: The first method works with Stable rust and requires the user the register the active message by implementing a runtime exported trait (LamellarAM) and calling a procedural macro (#lamellar::am]) on the implementation. The second method works on nightly Rust, but allows users to write serializable closures that are transferred and executed by the runtime without registration Second, Lamellar provides PGAS abstractions allowing users to allocate and operate on distributed arrays. Aside from the standard Put/Get operations (allowing remote nodes to read/write to memory on other nodes), Lamellar utilizes its Active Message framework to allow users to easily implement custom distributed reductions, by simply representing the reduction as a closure. In this talk we will provide a high level overview of the Lamellar Runtime, including examples that illustrate our communication primitives, as well as present some example benchmark implementations and results (e.g. triangle count, distributed histogram,...).

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MS106

Experiences Building Domain Specific Libraries for Irregular Applications over Openshmem

OpenSHMEM is a distributed, SPMD, one-sided communication model that facilitates asynchronous, fine grain communication among hundreds or thousands of processes. OpenSHMEM's flexibility means that it has found uses in a number of domains, from geophysics to high performance graph analytics. Like many distributed programming models in high performance computing, OpenSHMEM's programming model can be a barrier to entry for application developers that are more accustomed to higher level programming languages or models. It is rarely straightforward to translate high level operations (e.g. graph algorithms, sparse matrix operations) in to OpenSHMEM remote memory operations – and even when it is, doing a straightforward translation can yield suboptimal performance or scalability. However, building domain-specific libraries on top of OpenSHMEM allows users of leadership class computing facilities to leverage the scalability of OpenSHMEM while retaining high level programmability. This talk will discuss why OpenSHMEM's focus on irregular, fine grain, and asynchronous communication makes it fit-for-purpose for a wide range of application domains, including streaming graph analytics and data analytics/machine learning. We will walk through two case studies: (1) HOOVER, a DSL for distributed streaming graph modeling and analysis, and (2) SHMEM-ML, a DSL for distributed data analysis and machine learning.

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MS106

Legate NumPy: Accelerated and Distributed Array Computing

NumPy is a popular Python library used for performing array-based numerical computations. The canonical implementation of NumPy used by most programmers runs on a single CPU core and is parallelized to use multiple cores for some operations. In this talk we discuss Legate, a drop-in replacement for NumPy that requires only a single-line code change and can scale up to an arbitrary number of GPU accelerated nodes. Legate works by translating NumPy programs to the Legion programming model and then leverages the scalability of the Legion runtime system to distribute data and computations across an arbitrary sized machine.

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MS107

Time Evolution Problems for (2+1)-Dimensional Evolution Equations: Whitham Modulation Theory and its Applications

Whitham modulation theory has been applied with great success in large a variety of settings. Until recently, however, most studies were limited to (1+1)-dimensional systems, i.e., PDEs in one spatial dimension. In this talk I will show how a (2+1)-dimensional generalization of Whitham modulation theory can be used to derive the genus-1 Whitham modulation equations for the Kadomtsev-Petviashvili (KP) equation as well as other (2+1)-dimensional nonlinear evolution equations. I will then discuss some key properties of the resulting KP-Whitham system. Finally, I will show how the system can be successfully used to characterize analytically the time evolution of a variety of initial conditions, including soliton stems and a combination of solitons and a mean flow.

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MS107

Long-Time Asymptotics and Modulational Instability in Self-Focusing Media

Modulational instability, also known as Benjamin-Feir instability in the context of deep water waves, is one of the most ubiquitous phenomena in nonlinear science. The behavior of many modulationally unstable systems is governed by the focusing nonlinear Schrödinger equation on the line supplemented with some kind of nonzero boundary conditions at $\pm\infty$. This talk will discuss results on the long-time asymptotics of focusing NLS in the case of a generic class of symmetric nonzero boundary conditions by using the Deift-Zhou nonlinear steepest descent method for oscillatory Riemann-Hilbert problems. In the absence of discrete spectrum, it will be shown that the solution is given to leading order by a plane wave or by a modulated elliptic wave, depending on the value of the similarity ratio x/t. Moreover, in the case of discrete spectrum, the interaction between solitons and the aforementioned asymptotics will be characterized. Finally, numerical results for certain variations of focusing NLS will also be presented. This is joint work with Gino Biondini and Sitai Li.

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MS107

Numerical Inverse Scattering for the Periodic Problem for the KdV Equation

We consider forward and inverse scattering for the periodic problem for the Korteweg-de Vries (KdV) equation. Using well-known spectrum approximation techniques, we compute the scattering data for general initial data. The (generically) infinite-genus initial data is replaced with a genus g approximation with g large. The map from the scattering data to the solution is computed by solving a Riemann–Hilbert problem on $2g$ disjoint intervals. Fast linear algebra can be used to compute with $g \approx 1000$. The solution for the KdV equation can be computed for arbitrarily long times. Discontinuous initial data is also considered.

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MS108

Duality Gap Estimation via a Refined Shapley-Folkman Lemma

Based on a refinement of the Shapley-Folkman lemma and a finer characterization of the nonconvexity of a function, we propose a new estimate for the duality gap of nonconvex optimization problems with separable objective functions. We apply our result to a network flow problem and the dynamic spectrum management problem in communication systems as examples to demonstrate that the new bound can be qualitatively tighter than the existing ones. The idea is also applicable to cases with separable nonconvex constraints.

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MS108

Stability Analysis of Synchronization Patterns: Is Symmetry Really Your Friend?

Many biological and technological networks show intricate synchronization patterns, where several internally coherent but mutually independent clusters coexist. Which synchronization patterns we can ultimately observe are determined by their stabilities. It is widely believed that utilizing symmetries in the network structure is crucial to the characterization of a patterns stability. However, symmetry-based methods are limited in the types of synchronization patterns they can directly treat and can be computationally expensive. In this talk, I will show that when symmetry information is discarded, the stability problem becomes easier, not harder. By forgoing symmetry, we not only can analyze all synchronization patterns in a unified fashion but also develop algorithms that are orders of magnitude faster than symmetry-based ones. Our symmetry-independent method is based on finding the finest simultaneous block diagonalization of noncommuting matrices in the variational equation. This framework can be naturally extended to networks with generalized interactions, including hypergraphs and temporal networks.

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MS109

Trading Signals in VIX Futures

We propose a new approach for trading VIX futures. We assume that the term structure of VIX futures follows a Markov model. The trading strategy selects a multi-tenor position by maximizing the expected utility for a day-ahead horizon given the current shape and level of the VIX futures term structure. Computationally, we model the functional dependence between the VIX futures curves, the VIX futures positions, and the expected utility as a deep neural network with five hidden layers. Out-of-sample backtests of the VIX futures trading strategy suggest that this approach gives rise to reasonable portfolio performance, and to positions in which the investor can be either long or short VIX futures contracts depending on the market environment.

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MS109

When Uncertainty and Volatility are Disconnected: Implications for Asset Pricing and Portfolio Performance

We analyze an environment where the uncertainty in the equity market return and its volatility are both stochastic, and may be potentially disconnected. We solve a representative investor's optimal asset allocation and derive the resulting conditional equity premium and risk-free rate in equilibrium. Our empirical analysis shows that the equity premium appears to be earned for facing uncertainty, especially high uncertainty that is disconnected from lower volatility, rather than for facing volatility as traditionally assumed. Incorporating the possibility of a disconnect between volatility and uncertainty signi cantly improves portfolio performance, over and above the performance obtained by conditioning on volatility only.

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MS109

PCA for Implied Volatility Surfaces

Principal component analysis (PCA) is a useful tool when trying to construct factor models from historical asset returns. For the implied volatilities of U.S. equities there is a PCA-based model with a principal eigenportfolio whose return time series lies close to that of an overarching market factor. The authors show that this market factor is the index resulting from the daily compounding of a weighted average of implied-volatility returns, with weights based on the options' open interest (OI) and Vega. The authors also analyze the singular vectors derived from the tensor structure of the implied volatilities of S&P500 constituents, and find evidence indicating that some type of OI and Vega-weighted index should be one of at least two significant factors in this market.

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MS109

Statistical Consequences of Fat Tails: Real World Preasymptotics, Epistemology, and Applications

Switching from thin tailed to fat tailed distributions requires more than "changing the color of the dress". Traditional asymptotics deal mainly with either n=1 or n=8, and the real world is in between, under of the "laws of the medium numbers" –which vary widely across specific distributions. Both the law of large numbers and the generalized central limit mechanisms operate in highly idiosyncratic ways outside the standard Gaussian or Levy-Stable basins of convergence. A few examples: + The sample mean is rarely in line with the population mean, with effect on "naive empiricism", but can be sometimes be estimated via parametric methods. + The "empirical distribution" is rarely empirical. + Parameter uncertainty has compounding effects on statistical metrics. + Dimension reduction (principal components) fails. + Inequality estimators (GINI or quantile contributions) are not additive and produce wrong results. + Many "biases" found in psychology become entirely rational under more sophisticated probability distributions + Most of the failures of financial economics, econometrics, and behavioral economics can be attributed to using the wrong distributions.

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MT1

Optimal Transport for Machine Learning

This tutorial aims at presenting the mathematical theory of optimal transport (OT) and providing a global view of the potential applications of this theory in machine learning, signal and image processing. The first part of the tutorial will present the theory of optimal transport and the optimization problems through the original formulation of Monge and the Kantorovitch formulation in the primal and dual. The problem will be illustrated on simple examples. We will also introduce the OT-based Wasserstein distance and the Wasserstein barycenters that are fundamental tools in data processing of histograms. Finally we will present recent developments in regularized OT that bring efficient solvers and more robust solutions. The second part of the tutorial will present recent applications of OT in the field of machine learning. We will see how the mapping inherent to optimal transport can be used to perform domain adaptation. Finally we will discuss the use of OT on empirical datasets with applications such as generative adversarial networks and subspace estimation.

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MT1

An Introduction to Deep Generative Modeling

Deep generative models (DGM) are neural networks with many hidden layers trained to approximate complicated, high-dimensional probability distributions from a finite number of samples. When trained successfully, we can use the DGMs to estimate the likelihood of each observation and to create new samples from the underlying distribution. Developing DGMs has become one of the most hotly researched fields in artificial intelligence in recent years. The literature on DGMs has become vast and is growing rapidly. Some advances have reached the public sphere, for example, the recent successes in generating realistic-looking images, voices, or movies; so-called deep fakes. Despite these successes, several mathematical issues limit the broader use of DGMs: given a specific dataset, it remains challenging to design and train a DGM and even more challenging to find out why a particular model is or is not effective. To help students contribute to this field, this talk provides an introduction to DGMs and provides a concise mathematical framework for modeling the three most popular approaches: normalizing flows (NF), variational autoencoders (VAE), and generative adversarial networks (GAN). We illustrate the advantages and disadvantages of these basic approaches using numerical experiments. Our goal is to enable and motivate the reader to contribute to this proliferating research area. Our presentation also emphasizes relations between generative modeling and optimal transport.

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MT2

Tensor Decompositions: Applications and Algorithms

Tensor decompositions are generalizations of low-rank matrix approximations to higher dimensional data. They have become popular for their utility across applicationsincluding blind source separation, dimensionality reduction, compression, anomaly detectionwhere the original data is represented as a multidimensional array. Well highlight a few applications where tensor decompositions, such as CP and Tucker decompositions, are particularly effective. Well discuss properties of the various decompositions and guidelines for employing decompositions in different scenarios, and well describe the algorithms used to compute them.

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MT2

Topological Data Analysis: Computational Topology Tools for Data Science

The field of topology, within mathematics, has been around for centuries. For most of that time it was studied by theoretical mathematicians. But in the late 1990s and early 2000s researchers began to develop the field of Topological Data Analysis (TDA). The idea of TDA is that the “shape of data' can tell you interesting information about the data or system itself. In this tutorial I will provide topological background for TDA including the basic theory behind two of the most popular tools, persistent homology and mapper, along with brief code demos. I will give some examples of where TDA has been useful in real applications from understanding the space of natural images to detecting when certain kinds of machines are in proper working order. There will not be enough time to cover all of the exciting topics or applications of TDA but I hope to give you enough of a flavor of the field, along with plenty of references, to enable further exploration and application of these ideas.

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MP2

Numerical Predictions of Shear Stress and Cyclic Stretch in the Healthy Pulmonary Vasculature

Pulmonary hypertension due to left heart failure (PH-LHF) is a progressive disease associated with vascular remodeling. This study uses in-silico computational fluid dynamics of large and small pulmonary arteries and veins to predict wall shear stress (WSS) and cyclic stretch (CS), quantities serving as biomarkers for disease severity. We calculate dynamic blood pressure, blood flow, area deformation, WSS, and CS in the pulmonary circulation, providing a new way to investigate hypotheses related to disease progression.

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MP2

Continuous Dependence for Nonlocal Systems

Nonlocal models have gained interest due to their flexibility in handling discontinuities. In this poster we concentrate on the stability/continuous dependence of these for the nonlocal Poissons boundary value problem. We consider the stability of the solution with regards to changes in both a linear forcing term and a nonlinear forcing term, the collar (nonlocal boundary) term, and the kernel (a part of the operator itself that depicts the interactions between points).

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MP2

Lattice Point Counting: From Gauss Circle Problem to Heisenberg Norms

The question of how many integer lattice points are in, on, and near convex surfaces is a classical problem in number theory and other similar areas of mathematics. Beginning with the Gauss circle problem, the question of how many integer lattice points are in, on, and near convex surfaces has been rephrased over the years and expanded to include other surfaces. We will survey some of these variants and interesting proof techniques, such as tools in geometric measure theory. We conclude with a bound on the number of lattice points on and near a Heisenberg norm ball ($B_R^{\alpha,A} := \{(z,t) \in \mathbb{Z}^{2d}\, x\, \mathbb{Z} : |z|^\alpha + A|t|^{\alpha/2} \leq R^\alpha\}$), achieved by defining a measure on a thickened and truncated lattice. Our work was inspired by [A. Iosevich, K. Taylor, ”Lattice points close to families of surfaces, nonisotropic dilations and regularity of generalized Radon transforms.” New York Journal of Mathematics 17, pp. 811-828, 2011] and [R. Garg, A. Nevo, K. Taylor, ”The lattice point counting problem on the Heisenberg groups.” Ann. Inst. Fourier, Grenoble 65, 5, pp. 2199-2233, 2015]. We extend the method introduced by Iosevich and Taylor to allow for surfaces with points of vanishing curvature, such as the Heisenberg norm balls studied by Garg, Nevo, and Taylor.

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MP2

Three-Dimensional Structured-Tree Model for Predicting Fluid Dynamics in Pulmonary Arterial Networks with Pulmonary Hypertension

Pulmonary arteries form a rapidly branching network that serves to oxygenate blood. Pressure and flow can be determined by solving a multiscale 1D fluid dynamics model, where large arteries dimensions are taken from data and small vessels are represented by self-similar structured trees. This study uses a data-driven approach to obtain scaling factors and branching angles required to generate 3D structured trees. This allows us to predict perfusion in lungs with and without pulmonary hypertension.

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MP2

Metric Entropy and Nonlinear PDEs

Inspired by a question posed by Lax in 2002, the study of metric entropy for nonlinear partial differential equations has received increasing attention in recent years. This poster demonstrates methods to obtain sharp upper and lower bounds on the metric entropy for a class of real-valued bounded total variation functions [P. Dutta and K.T. Nguyen, Covering numbers for bounded variation functions, J. Math. Anal. Appl., 468, no. 2, 1131–1143, 2018] and then for a class of bounded total generalized variation functions taking values in a general totally bounded metric space [R. Capuani, P. Dutta and K.T. Nguyen, Metric entropy for functions of bounded total generalized variation, to appear in SIAM Journal on Mathematical Analysis, 2021 (https://arxiv.org/pdf/1912.00219.pdf)]. Thereafter we use each of these results to establish ε-entropy estimates for the set of viscosity solutions to the Hamilton-Jacobi equation with uniformly directionally convex Hamiltonian [S. Bianchini, P. Dutta and K.T. Nguyen, Metric entropy for Hamilton-Jacobi equation with uniformly directional convex Hamiltonian, 2020 (https://arxiv.org/pdf/2012.10577.pdf, submitted)] and the set of entropy admissible weak solutions to a scalar conservation law with weak genuinely nonlinear flux, respectively. Estimates of this type could provide a measure of the order of resolution of a numerical method required to solve the corresponding equation.

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MP2

Singular Limit and Global Stabilization of a PDE Model for Chemotaxis with Dynamic Boundary Conditions

We obtain global well-posedness and large-time behavior of a PDE model for chemotaxis with logarithmic sensitivity and logistic growth with dynamic boundary condition by imposing appropriate conditions on the boundary data. We show that there are boundary layer profiles for the singular diffusion limit similar to the Navier-Stokes equations boundary layer phenomena.

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MP2

Using Bayesian Inference to Learn the Role of Inhibitors in Blood Coagulation

Blood coagulation is a complex network of biochemical reactions involving positive and negative feedback. Positive feedback initiates the formation of blood clot and negative feedback stops its growth. Because both over-clotting and under-clotting result in serious, and sometimes deadly consequences, it is important to understand the regulation of coagulation by inhibitors. In this study, we investigate a specific coagulation inhibitor, tissue factor pathway inhibitor (TFPI), for which the mechanism of action is not fully understood. Previous mathematical models of TFPI have fit kinetic parameters to a single experimental time course but these models fail when applied to data from multiple experimental time courses simultaneously. We use Bayesian Inference to determine the posterior distribution of kinetic parameters by considering multiple experimental data sets simultaneously and to uncover the precise mechanism of action. Our likelihood framework is highly generalizable and will enable us to work toward a more complete understanding of inhibitors in coagulation.

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MP2

A Finite Horizon Optimal Stochastic Impulse Control Problem with a Decision Lag

We discuss an optimal stochastic impulse control problem in a finite horizon with a decision lag, by which we mean that after an impulse is made, a fixed number units of time has to be elapsed before the next impulse is allowed to be made. The continuity of the value function is proved. A suitable version of dynamic programming principle is established, which takes into account the dependence of state process on the elapsed time. The corresponding Hamilton-Jacobi-Bellman (HJB) equation is derived, which exhibit some special feature of the problem. The value function of this optimal impulse control problem is characterized as the unique viscosity solution to the corresponding HJB equation. An optimal impulse control is constructed provided the value function is given. Moreover, a limiting case with the waiting time approaching 0 is discussed.

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MP2

Lipid-Mediated Enzyme Reactions

Blood coagulation is a network of biochemical reactions whereby dozens of proteins act collectively to initiate a rapid clotting response. It is known that coagulation reactions are lipid-surface dependent, and this dependence is thought to help localize coagulation to the site of injury and enhance the association between reactants. Current mathematical models of coagulation fail to agree with laboratory studies under variations in lipid concentrations. In particular, models overestimate conversion efficiencies of critical coagulation proteins, specifically the prothrombin-thrombin reaction pathway. We developed a a mathematical model of lipid-mediated enzyme reactions where the association rate between lipid-bound reactants are modified by an interaction probability. The interaction probability is derived by considering the fraction of the lipid surface that is occupied by any lipid-bound species, and accounts for surface crowding. Preliminary model results agree with experiments and reveal a critical lipid concentration where the rate of prothrombin conversion is maximized, inferring that the model can describe the dilution effect where, as lipid is increased, proteins are physically separated, and reaction rates decrease.

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MP2

Characterizing Absorbing Sets using Syndromes and Cosets

Absorbing sets are combinatorial structures in a codes Tanner graph that have been shown to characterize iterative decoder failure of LDPC codes. This poster examines the connection between absorbing sets and the syndromes of their support vectors. We provide a new characterization of fully absorbing sets and show how sets of absorbing set support vectors appear as translates of codewords in a codes subspaces. These techniques are used to derive new absorbing set search methods.

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MP2

Convergence of Nonlinear Nonlocal Operators to Classical Counterparts

Nonlinear diffusion models phenomena where diffusivity is temperature or concentration dependent. Nonlocal operators can model effects that classical partial differential systems cannot capture. Combining the two, we consider nonlinear nonlocal models. In particular, showing that the action of a nonlocal operator localizes to the analogous classical operator and that solutions to a nonlocal boundary value problem converges to the classical solution.

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MP2

Pulsing and Photosynthesis: Numerical Simulations of Soft Corals

Corals in the family Xeniidae actively pulse their tentacles. It is hypothesized that the pulsing mixes the fluid to facilitate the photosynthesis of the symbiotic algae on their tentacles. Numerical simulations of the resulting fluid flow of a pulsing soft coral, using the immersed boundary method, coupled to a novel photosynthesis model will be presented. The benefit of pulsing for mixing and photosynthesis in different parameter regimes is quantified to gain insight into this behavior.

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MP2

Optimal Control in Fluid Flows through Deformable Porous Media

We consider an optimal control problem subject to a nonlinear poro-visco-elastic model with applications to fluid flows through biological tissues. In particular, our goal is to optimize the fluid pressure using either distributed or boundary control. We present results on the existence of optimal control and the associated necessary optimality conditions.

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MP2

Bilinear Control of Parabolic Evolution Equations

Despite the importance of control systems governed by bilinear controls for the description of phenomena that could not be modeled by additive controls, such as for instance the vibration of a beam composed by *smart materials*, or the process of increasing the speed of a chemical reaction by adding *catalysts*, the action of multiplicative controls is generally not so widely studied as it happens for boundary and locally distributed controls. The main reasons of this fact might be found in the intrinsic nonlinear nature of such problems and furthermore, for controls that are scalar functions of time, in an ineluctable obstruction for proving results of classical exact controllability which is contained in the celebrated work of Ball, Marsden and Slemrod (1982). In this poster I will present results, obtained in collaboration with F. Alabau-Boussouira and P. Cannarsa, of stabilization and controllability of evolution equations of parabolic type via bilinear control to some particular target trajectories called *eigensolutions*. Moreover, I will show the application of our abstract results to parabolic equations such as the heat equation with Dirichlet or Neumann boundary conditions, degenerate parabolic equations and furthermore to diffusion equations on a network structure.

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MP2

Frictionless Indentation of a Rigid Stamp into a Half-Space

Material properties at nanoscale exhibit size-dependent behavior which can be attributed to the influence of surfaces and interfaces on the properties of materials. Due to this, contact problems at nanoscale have to take into account surface energy. In this talk, we consider an isotropic half-space subjected to nanoscale contact with a rigid punch. The surface energy in the Steigmann-Ogden form is used to model the surface of the half-space while linear elasticity is used to model the bulk of the material. The nanoindentation problem is solved using Boussinesqs displacement potentials and Hankel integral transforms. The problem is reduced to a single integral equation, the character of which is studied, and a numerical method of solution to the corresponding integral equation using Gauss-Chebyshev quadrature is presented.

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MP3

Analysis of a Foragers Decision-Making Heuristic

Optimal foraging theory favors ecological behavior that maximizes long term caloric gains over time, and laboratory observations indicate that decisions for such long-term maximization are impulsive and depend on minimal information. We posit that if the foragers current energy state is less than the preys profitability, then the forager will consume the prey. Otherwise, the forager continues searching. We will prove that this decision-making heuristic optimizes the forager's energy state through a proof of convergence in mean. Faculty Advisors: Theodore Pavlic, Professor, tpavlic@asu.edu; Naala Brewer, Lecturer, nbrewer@asu.edu

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MP3

Comparing Numerical Solution Methods for the Cahn-Hilliard Equation

In this presentation, we will consider numerical methods based on the convexity splitting technique to solve the Cahn-Hilliard equation, a model for phase separation, with periodic boundary conditions. These methods include linear extrapolation, second-order backward difference formulas, and implicit-explicit Runge-Kutta methods. The Cahn-Hilliard equation, which is derived from a gradient flow of an energy functional, is a higher-order, parabolic nonlinear partial differential equation. As such, each of the proposed solvers preserves the energy decreasing property of this equation. The solution methods, which were implemented using fast Fourier transformations, were compared by means of accuracy and computational runtime. Furthermore, the convexity splitting parameter was varied in order to observe its effects on the accuracy and stability of numerical solvers. The best method for modest accuracy was determined to be the first-order linear extrapolation method. The preferred higher-order solver was an implicit-explicit Runge-Kutta scheme with relatively low computational cost. Simulations confirmed that this method preserves stability at larger timesteps while maintaining a high degree of accuracy at both large and small timesteps. This method can be extended to the 3D form of the Cahn-Hilliard equation for applications, such as modeling tumor growth. Faculty Advisors: Saulo Orizaga, New Mexico Tech, saulo.orizaga@nmt.edu

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MP3

Developing Computational Models to Detect Radiation in Urban Environments

The main objective of this project is to detect, characterize, and locate radioactive sources in urban environments using computational models based on machine learning and statistical techniques. The project explores multiple approaches such as signal processing methods, and neural networks. Unnatural radiation sources, such as Uranium or Plutonium, can compromise the safety of the population if they remain undetected by radiological search and response teams. Moreover, the computational model being developed must be capable of identifying the type of radiation source, classifying it as innocuous (i.e., isotopes used in medical and industrial settings) or harmful (nuclear weapons). The project is currently supported by the Pacific Northwest National Laboratory (PNNL), in collaboration with the Department of Mathematics at Embry-Riddle. Faculty Advisors: Mihhail Berezovski, Assistant Professor of Mathematical Sciences, berezovm@erau.edu

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MP3

Comparing Finite-Time Lyapunov Exponents and Lagrangian Descriptors for Identifying Phase-Space Structures in Two-Dimensional Double-Gyre Flow

In this presentation we will compare the advantages, limitations, and computational considerations of using Finite-Time Lyapunov Exponents (FTLEs) and Lagrangian Descriptors (LDs) as tools for identifying phase-space structures in two-dimensional time-periodic flows. These structures include mechanisms of transport and mixing present in oceanic flows, and the methods have been recently applied to other dynamical systems such as in chemical reaction dynamics. We specifically use these tools to study the stable and unstable manifolds of hyperbolic stagnation points, and the Kolmogorov-Arnold-Moser (KAM) tori associated with elliptic stagnation points. The background and theory of both FTLEs and LDs will be presented, and examples of both methods will be shown based on a simplified two-dimensional version of double-gyre flow, which is a feature of large-scale ocean circulation. Faculty Advisors: Kevin McIlhany, United States Naval Academy, mcilhany@usna.edu

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MP3

Let Optimization be Your Guide for a Magical Family Trip in Disneyland Paris

Disneyland is a magical place for young and old alike. Yet the size of the park, the age restrictions of the attractions, the preferences amongst different age groups and the time a family could spend in the park, makes it difficult to decide which attractions to visit. In order to simplify this complication, we start by collecting data from the Disneyland Paris website and other reliable sources which include ratings of the attractions for each age group and we formulate an Orienteering Problem that aims to find the route achieving the maximum total rating. Our case study tries to answer two questions: (i) how each family member should individually navigate the park maximizing his/hers total rating, and (ii) how a family as a single group should navigate the park such that all family members achieve their goals. Our results show that if the family stay as a single group, the loss in total rating is negligible compared to each family member navigating the park individually. Faculty Advisors:, Angelos Georghiou, University of Cyprus, angelos.georghiou@gmail.com

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MP3

Near-Optimal Histogram Testing

Histograms are probability distributions with piecewise constant probability mass function: if the mass function is piecewise constant on k intervals, the distribution is said to be a k-histogram. When dealing with large datasets, histograms are one of the most common ways to represent data succinctly. We study the following testing problem: given i.i.d. samples from an unknown distribution p supported on 1, 2, ..., n, one must distinguish between the cases that p is a k-histogram versus far from any k-histogram in total variation (statistical) distance. Our main contributions are an efficient testing algorithm whose sample complexity is optimal, within logarithmic factors, and a nearly matching sample complexity lower bound; both improving on the previous state-of-the-art. Faculty Advisors: Ilias Diakonikolas, University of Wisconsin Madison, ilias.diakonikolas@gmail.com; Clment Canonne, University of Sydney, clement.canonne@sydney.edu.au

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MP3

Predictive Analytics for Dynamic Pricing in Private Aviation

The method of predicting private flight demand exists only as a manual process, resulting in restrictions with time and overall efficiency. In the private aviation industry, dynamic pricing is a tool used to help computerize the flight demand predictions as it decreases time consumption in the procedure, increases company revenue while maintaining competitiveness in the industry and improves customer satisfaction. OneSky Network, the IT branch of a private jet company located in Embry-Riddle Aeronautical Universitys Micaplex, teamed up with a few students at Embry-Riddle Aeronautical University for a research project that explores the concept of dynamic pricing with the ultimate goal of implementing such an algorithm for the private aviation industry. The objective of this research project is to create prediction models that will accurately predict private flight demand over the course of a year using three years of historical flight data that were provided by OneSky. Support for this project is provided by the National Research Experience for Undergraduates Program (NREUP) of the Mathematical Association of America funded by the NSF Grant #1950644. Faculty Advisors: Mihhail Berezovski, Embry-Riddle Aeronautical University, berezovm@erau.edu

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MP3

Money Managers Portfolio Relations. Evidence from South Africa

This paper explores the hypothesis that money managers and prospective investors exchange information and ideas about assets to one another directly, through word-of-mouth communication. Our sets of hypotheses appear as follows; Based on location, a mutual Fund manager is more likely to buy (or sell) a particular stock in any quarter if other managers in the same city are buying (or selling) that same stock. This pattern shows up even when the Fund manager and the stock in question are located far apart. On gender basis, a male Fund manager is more likely to relate his investment style to other male managers in his lines and the same is true for the female counterparts. Lastly, based on race, white managers do spread market trading information faster than the black mangers due to some factors. The evidence to all these above conjectures can be interpreted in terms of an epidemic model in which investors spread information about stocks to one another by word of mouth. Thus, this study employs an epidemic approach to modelling the word of mouth information transmission among various mutual Fund managers, with effect analysis on market performance and behaviour. Faculty Advisors: Mashasha Maxwell

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MP3

Discrepancy-Based Inference for Intractable Gen-

erative Models using Quasi-Monte Carlo

Intractable Generative models are models for which the likelihood is unavailable but sampling is possible. Most approaches to parameter inference in this setting require the computation of some discrepancy between the data and the generative model. This is for example the case for minimum distance estimation and approximate Bayesian computation. These approaches require sampling a high number of realisations from the model for different parameter values, which can be a significant challenge when simulating is an expensive operation. In this paper, we propose this approach by enforcing "sample diversity" in simulations of our models. This will be implemented through the use of quasi-Monte Carlo point sets. Our key results are sample complexity bounds which demonstrate that this approach can significantly reduce the number of samples required to obtain a given level of accuracy when using three of the most common discrepancies in this field: the maximum mean discrepancy, the Wasserstein distance, and the Sinkhorn divergence. Faculty Advisors: Francois-Xavier Briol, University College London, f.briol@ucl.ac.uk

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MP3

Analysing Early Warning Signals of Disease Elimination by Approximating the Potential Surface

The theory of critical slowing down states that a system displays increasing relaxation times as it approaches a critical transition. Such changes in relaxation times can be seen in statistics generated from data timeseries, which can be used as early warning signals of a transition. While analytic equations have been derived for various early warning signals in a variety of epidemiological models, there is frequent disagreement with the general theory of critical slowing down, with some indicators performing well when used in prevalence data but not when applied to incidence data. We investigate this effect in an SIS model by reconstructing the potential surface for different types of data. By modelling prevalence, incidence and the rate of infection as stochastic differential equations, then using an equation-free method to approximate their drift functions from simulated timeseries, we reconstruct the potential surface for each data type. Slowly varying parameters provides insight into how the shape of the potential surface changes. Analytic equations for the drift functions are also derived for comparison with simulated results, showing that the potential surface for all data types becomes shallower upon the approach to a critical transition from either direction, as predicted by critical slowing down. Faculty Advisors: Louise Dyson, University of Warwick, l.dyson@warwick.ac.uk

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MP3

Building an Artificially Intelligent Player to Play Settlers of Catan

In recent years, the abilities of Chess and Go playing artificial intelligences has increased greatly to become superior to most human competitors, but this focus has rarely been turned toward specialist games. This project is aimed at creating a competent game playing AI in the game of Settlers of Catan. In attempting to replicate the artificial intelligences that were created to play Chess and Go, this project will analyze what is needed for a computer to play the game efficiently and at a high level. While Chess and Go utilize simpler boards and options in game, Settlers of Catan offers a large amount of decisions every turn that can be explored that would de-incentivize a brute force method of computation. By taking advantage of the board design, the strict turn order, and the expanding options of play as the game goes on, the computer intelligences could compete better than random choice and standard human players. Faculty Advisors: Quan Tran, University of Science and Arts of Oklahoma, qtran@usao.edu

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MP3

Best Strategy for Each Team in the Regular Season to Win Champion in the Knockout Tournament

In J. Schwenk.(2018) What is the Correct Way to Seed a Knockout Tournament? Retrieved from The American Mathematical Monthly, Schwenk identified a surprising weakness in the standard method of seeding a single elimination (or knockout) tournament. In particular, he showed that for a certain probability model for the outcomes of games it can be the case that the top seeded team would be less likely to win the tournament than the second seeded team. This raises the possibility that in certain situations it might be advantageous for a team to intentionally lose a game in an attempt to get a more optimal (though possibly lower) seed in the tournament. We examine this question in the context of a four team league which consists of a round robin regular season followed by a single elimination tournament with seedings determined by the results from the regular season. Using the same probability model as Schwenk we show that there are situations where it is indeed optimal for a team to intentionally lose. Moreover, we show how a team can make the decision as to whether or not it should intentionally lose. We did two detailed analysis. One is for the situation where other teams always try to win every game. The other is for the situation where other teams are smart enough, namely they can also lose some games intentionally if necessary. The analysis involves computations in both probability and (multi-player) game theory. Faculty Advisors: Jonathon Peterson, Purdue University, Department of Mathematics, peterson@purdue.edu

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PP1

Computational Simulation of Patterns in a Reaction-Difussion Model

Recent studies in reaction-diffusion models have been oriented to produce patterns for studying polycrystalline materials as graphene oxide. Here we show an algorithm to obtaining patterns from a reaction-diffusion equation. Results suggest that it is possible to obtain theoretical patterns from the reaction-diffusion equation, as expected, compared with the experimental patterns of high-resolution transmission electron microscopy (HR-TEM) in graphite oxide samples.

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PP1

LGN-CNN: a Biologically Inspired CNN Architecture

In our work, we introduce a biologically inspired Convolutional Neural Network (CNN) architecture called LGN-CNN, that has a first convolutional layer composed by a single filter and that mimics the role of the Lateral Geniculate Nucleus (LGN). Then we investigate the retinex effect induced by this filter. The presence of an unique filter induces rotational invariant properties of the network, so that the lerned filter shows a rotationally symmetric pattern and turns out to be a good approximation of a Laplacian of Gaussian (LoG) and of receptive profiles (RPs) of the cells in the LGN. In this way we establish a strong analogy between our LGN-CNN and the visual system structure. We give computational results, and investigate the contrast invariance capability of the LGN-CNN, comparing the Retinex effects of the first layer of LGN-CNN and the Retinex effects of a LoG. Finally, we compare the statistics of filters of the second layer with the biological distribution of recorded RPs of simple cells in the Primary Visual Cortex. The similarity we find enforces the analogy between our architecture and the structure of the first layers of the visual system. A preprint on this topic is available at https://arxiv.org/abs/1911.06276.

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PP1

The Select Boost Algorithm Improves Variable Selection in Linear Models

With the growth of big data, variable selection has become one of the critical challenges in statistics. Although many methods have been proposed in the literature their performance in terms of recall and precision are limited in a context where the number of variables by far exceeds the number of observations or in a highly correlated setting. We propose a general algorithm which improves the precision of any existing variable selection method. This algorithm is based on highly intensive simulations and takes into account the correlation structure of the data. The user of selectBoost can use this algorithm to produce a confidence index or choose an appropriate precision-selection trade-off to select variables with high confidence and avoid selecting non-predictive features. The main idea behind our algorithm is to take into account the correlation structure of the data and thus use intensive computation to select reliable variables. We succeeded in improving the precision of the lasso selection method with relative stability on recall and F-score and we demonstrate the performance of our algorithm on both simulated and real data for linear models. The select boost algorithm is available on the CRAN as an R package.

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PP1

Viscoelastic Flows with First-Order Conservation Laws and Relaxation

We propose a system of first-order conservation laws with relaxation (i.e. a system of balance laws) for the compressible non-isothermal viscoelastic flows of Maxwell fluids, possibly heat-conducting following the Maxwell–Cattaneo law. By establishing a strictly convex mathematical entropy, the system is shown symmetric-hyperbolic. The prominent feature of the proposed model is the short-time existence and uniqueness of smooth solutions that are genuinely causal (perturbations of uniform flows propagate at finite speed). Viscoelastic flows of Maxwell fluids with conservation laws, Sebastien Boyaval, ESAIM: M2AN, https://doi.org/10.1051/m2an/2020076

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PP1

Seamless Numerical Homogenization for Multiscale Problems

Many numerical methods inspired by analytic averaging theory for dynamical systems or homogenization theory for elliptic operators require scale separation between the small and large scales in the problem. Recently some techniques for dynamical systems have been proposed to mitigate this restriction, such as the Seamless Multiscale Method [E, Ren, Vanden-Eijnden, A general strategy for designing seamless multiscale methods] and FLAVORS [Tao, Owhadi, Marsden, Non-intrusive and structure preserving multiscale integration of stiff ODEs, SDEs and Hamiltonian systems with hidden slow dynamics via flow averaging]. We establish a rigorous link between multiscale dynamical systems and one-dimensional homogenization, which implies a seamless multiscale framework also for numerical homogenization. This framework is then generalized to higher dimensions. Analysis and numerical examples show desirable properties of the proposed technique as well as the broad scope of application. This framework also works with partial observations of the system. A practical component is preprocessing by scale detection, for example by, empirical mode decomposition or Synchrosqueeze algorithms.

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PP1

Cpfloat: A C Library for Emulating Low-Precision

Arithmetic

Low-precision floating-point arithmetic can be simulated via software by executing each arithmetic operation in hardware and rounding the result to the desired number of significant bits. For IEEE-compliant formats, rounding requires only standard mathematical library functions, but handling subnormals, underflow, and overflow demands special attention, and numerical errors can cause mathematically correct formulae to behave incorrectly in finite arithmetic. Moreover, the ensuing algorithms are not necessarily efficient, as the library functions these techniques build upon are typically designed to handle a broad range of cases and may not be optimized for the specific needs of floating-point rounding algorithms. CPFloat is a C library that offers efficient routines for rounding arrays of binary32 and binary64 numbers to lower precision. The software exploits the bit level representation of the underlying formats and performs only low-level bit manipulation and integer arithmetic, without relying on costly library calls. In numerical experiments the new techniques bring a considerable speedup (typically one order of magnitude or more) over existing alternatives in C, C++, and MATLAB. To the best of our knowledge, CPFloat is currently the most efficient and complete library for experimenting with custom low-precision floating-point arithmetic available in any language.

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PP1

Repeated Measures Analysis of Natural Killer Cell Data at the 50% Cytotoxicity Level

A repeated measures analysis of natural killer cell data is conducted. The SAS/STAT (2018) procedure proc mixed was used for the repeated measures analysis. The immune parameter of interest is the natural killer cell values obtained for an input 50% cytotoxicity level [NK50]. The original study was carried out at the University of California San Francisco. SAS software functions were used to simulate stress and health data by randomly selecting observations on a sample of subjects to demonstrate methodology. Simulations based upon summary data and models fit to the data were used for representative data. Two types of stress outcome are examined. These are the acute (short-term) stress and chronic (long-term) stress levels. The grouping variables used include gender, employment status and a cluster variable obtained from a cluster analysis of nine mood variables. A principal component analysis is used on sets of (NK100, NK50, NK25, NK12, NK6) sequences of data. The NK100, NK50, NK25, NK12 and NK6 are the natural killer cell values obtained for input 100%, 50%, 25%, 12.5% and 6.25% cytotoxicity levels, respectively. Models often used in predicting cytotoxicity values involve an exponential fit (Archontoulis and Miguez, 2014). Models are fit to the data to obtain estimates of the NK50 using the modified Gauss Newton to obtain parameter estimates for the exponential growth model.

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PP1

Effectivity of Crowd-Sourcing Functional Connectivity Network Inference Methods of fMRI Data

Understanding brain network interactions is one step towards understanding behavior, cognition, and various neurological disorders. Functional MRI (fMRI) scans are a source of information to infer such network interactions. In the neuroscience community, there are several methods based on say, correlation, coherence, mutual information to deduce functional connectivity networks. Sometimes, these methods on their own may lead to false positives or give partial network connectivity results. In this work, we explore the utility of crowd-sourcing inference methods to obtain more accurate network connectivity maps. To that end, we utilize a rich dataset of around 1400 fMRI timeseries generated from 28 different networks [Smith et al., 2011]. The results of the poster show that, in the absence of a gold standard, rather than using a single reverse-engineering method, it is more prudent to use a combination of high-performing methods.

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PP1

Machine Learning Assisted Chimera and Solitary States in Networks

Chimera and Solitary states have captivated scientists and engineers due to their peculiar dynamical states corresponding to co-existence of coherent and incoherent dynamical evolution in coupled units in various natural and artificial systems. In this work, using supervised machine learning, we predict (a) the precise value of delay which is sufficient for engineering chimera and solitary states for a given set of system's parameters, as well as (b) the intensity of incoherence for such engineered states. Ergo, using few initial data points we generate a machine learning model which can then create a more refined phase plot as well as by including new parameter values. We demonstrate our results for two different examples consisting of single layer and multi layer networks. First, the chimera states (solitary states) are engineered by establishing delays in the neighbouring links of a node (the interlayer links) in a 2-D lattice (multiplex network) of oscillators. Then, different machine learning classifiers, K-nearest neighbours (KNN), support vector machine(SVM) and multi-layer perceptron neural network (MLP-NN) are employed by feeding the data obtained from the network models. Once a machine learning model is trained using the limited amount of data, it predicts the precise value of critical delay as well as the intensity of incoherence for a given unknown systems parameters values.

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PP1

Two-Dimensional Laminar Flow of the Generalized Fluid Across an Unconfined Inclined Square Cylinder using Finite Element Methods

The work concerns a least-squares finite element method (LSFEM) for the power-low generalized fluid flow across a square cylinder. The LSFEM method offers the advantages of always generating a symmetric positive definite system, insensitivity to equation type, and no need for compatibility conditions between finite element spaces. This can be accomplished using low-order basis functions without substantial complications in coding. The LSFEM uses the L^2-norm of the residuals of each equation multiplied by appropriately adjusted weights. Numerical results indicate that we can apply the LS method to flow problems and obtain the drag coefficients, viscosity, and velocity. The effects of the power-law index have been investigated in the steady flow regime. These results agree with others published in the literature. Hence, we obtain that the LSFEM in non-Newtonian fluid simulations with shear-thinning and shear-thickening characteristics.

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PP1

A New Algorithm for Reverse-Engineering Patterned Heterogenous Networks

We created a new algorithm dedicated to biological network reverse-engineering that allows for single or joint modelling of, for instance, genes and proteins. It is designed to work with patterned data. Famous examples of problems related to patterned data are: recoveringsignalsin networks after astimulation(cascade network reverse engineering) and analysingperiodic signals. The algorithm begins with a step to select the actors that will be used in the reverse engineering upcoming step. An actor can be included in that selection based on itsdifferential effects (for instance gene expression or protein abundance) or on its time course profile. The actors are then clustered and various time-varying patterns of interaction between the clusters can be specified. Manyinference functions can be used in the inference step of the algorithm. They are dedicated to getting specific features for the inferred network such as sparsity, robust links, high confidence links or stable through resampling links. In order to include biological a priori knowledge in the network inference, we wanted to enable weighted inference and had to extend some known algorithm such as stability selection. We will provide examples of the use of the algorithm on simulated data or on real microarray or RNA-Seq data.

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PP1

Modeling of Cooperative Associations in Harvester Ant, *Pogonomyremx Californicus*

The understanding and study of the evolution of cooperation present a challenge in biological studies, especially among non-relatives. For non-relatives, indirect benefits have no payoff or relevance for individuals since in a system of non-relatives, group selection occurs as opposed to individual selection. In these systems, cooperation evolves as a result of a group-level advantage. There are few examples of group-level selection found in nature. Among these few examples are the species of the harvester ant *Pogonomyremex californicus*. These ants provide an ideal example for study since they consist of newly mated queens who either primarily found nests alone or form cooperative groups of non-relatives to establish nests. There is experimental data on these ants that have shown a group-level advantage among cooperator ants. I will create an agent-based model that incorporates both lab and field data in order to analyze the amplification and damping of different phenotypes. In addition to cooperators and noncooperators, I will add a cheater phenotype to see if they will affect the system and if the cooperator phenotype will prevail. I hope to create a realistic agent-based model that addresses the question of how social phenotypes are shaped by the transition to cooperative associations.

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PP1

Confidence Assessment using Optimal Feature and State Characterization for an In-Situ Phosphate Level Time Series Array

The ability to understand riverine phosphate level spatial structure is important for the comprehension of baseline pollutant dynamics of watersheds from which anomalous system behavior can be assessed. This comprehension in turn impacts water quality evaluation, sanitation, and public health. Acquired riverine phosphate measurements taken at three sites in the Mississippi watershed stretching from fall 2016 to summer 2018 allow the opportunity to examine site dimensional structure of phosphate levels via Bayesian and manifold learning algorithms. More importantly, such techniques allow for the development of a confidence assessment methodology based on optimized parameter learning and state prediction which includes Gaussian mixture modeling, Laplacian eigenmaps, and Gaussian processes. Preliminary machine learning statistical results demonstrate a formulism in which future data points can be assessed or judged as anomalous or not conditioned on the optimal modeling of the spatio-temporal variability and structure of old training data. The data processing technique shows great promise for the creation of an ensemble algorithmic approach to optimal confidence assessment of complex system data.

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PP1

Multiparameter Full Waveform Inversion and Optimal Transport

Full waveform inversion (FWI) is a powerful computational tool in seismic imaging and widely used to determine high resolution of subsurface properties in seismology today. FWI is a PDE constrained optimization technique. The traditional misfit or objective function in this optimization is the L2 norm. Earlier the Wasserstein metric from optimal transport has proved to be a superior choice for misfit function in many situations. Properties as, for example, convexity and insensitivity to noise were established in theory and in practice. This was the case for a single parameter wave equation with inversion for the wave velocity. The multiparameter case is much more challenging with finding both density and bulk modulus. This will require matching amplitudes in refractions in the recorded signals and not just travel time. Earlier results of applying the Wasserstein metric to problem of velocity recovery below a reflecting surface clearly indicate that the Wasserstein metric is sensitive to amplitude variations. In this project we are investigating the performance in the multiparameter setting based on finite difference wave equation approximations. The preliminary numerical results indicate that the Wasserstein metric is a very promising choice of misfit function for FWI in the multiparameter case.

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PP1

Diagnosing Respiratory Illness Deterioration Using Machine-Learning Classifiers Trained on Simulated Patient Vignettes

Viral and chronic respiratory illnesses are responsible for \$100s of billions in global healthcare utilization and 10s of millions of deaths annually. While the recent Covid-19 pandemic has been a singular phenomenon leaving more than 107M confirmed cases and 2.3M deaths (as of February 2021) in its wake, chronic Lung Disease (primarily Asthma and COPD) and seasonal influenza have persisted for decades as a source of nearly \$1 trillion in annual health expenditures and millions of global deaths. The particular event that drives the majority of healthcare spending and morbidity among these illnesses is a rapid health deterioration episode that manifests as either emergency care (in the case of chronic lung disease) or rapid infection spread (in the case of Covid-19 and Influenza). In this study, we present a machine-learning approach to identifying clinically significant flare-ups of respiratory illness using globally available clinical characteristic data. The methodology leverages Bayesian Inference and Monte Carlo methods to generate representative patient scenarios from marginally distributed health severity data and train triage algorithms. Machine-learning prediction models are evaluated in out-of-sample validation tests of accuracy, sensitivity, specificity, ppv, and npv when detecting health deterioration and recommending the most appropriate responsive care.

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PP1

Hemodynamics in Hypoplastic Left Heart Syndrome Patients Assessed with a 1D Arterial Network Model

Patients with cardiovascular disease experience physiologic changes in their heart, large vessels, and peripheral vessel networks. An example is hypoplastic left heart syndrome (HLHS), a disease in which the left side of the heart is underdeveloped leaving patients with only one functioning ventricle. Treatment of HLHS involves reconstructing the aorta removing it from the left ventricle and attaching it to the right ventricle. This initial reconstruction is the first step in a series of surgeries that lead to a Fontan circulation; a circuit that allows patients to live with univentricular circulation. While patients survive into adulthood, most experience cardiovascular problems including reduced cardiac output leading to insufficient cerebral perfusion. Current clinical assessments are made from analysis of 4D MRI images quantifying 3D flow patterns in the aorta. However, these do not provide information about energy loss, wave-intensity, or cerebral perfusion. This study uses 1D arterial network model computing these quantities in patients with HLHS. To investigate the effects that vascular remodeling has on perfusion, predictions will be compared to a single ventricle control patient; a patient with double outlet right ventricle (DORV), for which the aorta does not have to be reconstructed. Outputs include pressure and flow predictions in vessels of the systemic system for patients at supine rest and upright exercise as well as wave-intensity analysis.

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PP1

Premelting Controlled Active Matter in Ice

A collection of self-propelled particles can undergo complex dynamics due to hydrodynamic and steric interactions. In the case of a foreign particle inside a subfreezing solid, such as a particle in ice, a premelted film can form around it allowing the particle to migrate under the influence of an external temperature gradient, which is a phenomenon called *thermal regelation*. It has recently been shown that the migration of particles of a biological origin can accelerate melting in a column of ice and thereby migrate faster. We have previously shown that the effect of regelation plays a major role in the migration of inert particles and impurities inside ice, with important environmental implications. In particular, the question of how the activity affects a particles position over time is essential for paleoclimate dating methods in ice cores. We re-cast this class of regelation phenomena in the stochastic framework of active Ornstein-Uhlenbeck dynamics and make predictions relevant to this and related problems of interest in geophysical and biological problems.

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PP1

A Dynamic Inflammatory Response Model for Bolus Versus Continuous Administration of Endotoxin

Uncontrolled, persistent inflammation is a hallmark of individuals with medical conditions such as sepsis, a leading cause of death in U.S. hospitals. While a bolus administration of lipopolysaccharide (LPS) to healthy volunteers is a common short-term inflammation model, a continuous infusion of LPS over an extended time frame better represents the sustained inflammation present in conditions like sepsis. A number of studies have used mathematical modeling to examine the inflammatory feedback in response to a bolus administration of endotoxin, and these models were validated against bolus murine and human data. Analysis of bolus versus continuous administration of endotoxin data reveals that a continuous administration of LPS results in delayed peaks of pro and anti-inflammatory cytokines and increases in peak magnitude of TNF-α and IL-10. To further the understanding behind these differences, we adapt a 2 ng/kg bolus-dose inflammatory response model formulated as a system of ordinary differential equations tracking selected cytokines and cells to study the inflammatory response to a continuous infusion of endotoxin over an extended period of time. Using sensitivity analysis and parameter estimation, we validate the model using experimental data from a study where 2 ng/kg of LPS is administered over a 4-hour period in nine healthy volunteers.

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PP1

Parameter Estimation in Branching Random Walks

Branching random walks are used to model a variety of phenomena in biological systems. We consider a simple branching random walk model, originally introduced in the study of dendritic growth, and introduce analytic results on the branching parameter. We compare parameter estimation techniques that utilize the analytic results and describe their sensitivity to a number of variables. We will also show how the techniques we develop can be utilized when exact analytic results are not attainable.

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IP1

Shortest Path Algorithms for Road Navigation

Computer-generated driving directions are commonplace nowadays. Efficient shortest path and distance oracle algorithms for road networks are one of the main enablers of modern navigation systems. We discuss the evolution of these algorithms for the last three decades. In particular, we discuss ideas that lead to speed-ups of over three orders of magnitude. We also discuss incorporation of real-world constraints and algorithmic extensions, which make driving directions more precise and easier to use in the real world.

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IP2

Matrix-Free Jacobian Chaining

Algorithmic Differentiation (AD) yields tangent and adjoint versions of differentiable programs. Known Jacobians of a set of elemental functions are multiplied according to the chain rule of differentiation. Tangent [adjoint] programs evaluate matrix-free products of the [transposed] Jacobian with a given matrix. Modular AD views on large-scale numerical simulation programs can be represented as directed acyclic graphs with edges representing (partial) Jacobians of individual subprograms. The combinatorial optimization problem aiming to accumulate the Jacobian of the entire program with minimal computational cost turns out to be intractable. Matrix-free Jacobian chain products represent a relevant special case. They are defined in terms of tangents and adjoints of individual modules. In this talk we discuss several variants of the Matrix-Free Jacobian Chaining problem. We propose a dynamic programming solution for the unconstrained case. Bounds on the available persistent memory (required by the adjoint) make the problem computationally intractable. Our results represent an important step towards rigorous AD mission planning.

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IP3

Combinatorial Optimization Algorithms for Clustering and Machine Learning

Algorithms for machine learning tasks fall most often in the realm of AI or continuous optimization of intractable problems. We present combinatorial algorithms for machine learning, data mining, and image segmentation that, unlike the majority of existing machine learning methods, utilize pairwise similarities. These algorithms are efficient and reduce the classification problem to a network flow problem on a graph. One of these algorithms addresses the problem of finding a cluster that is as dissimilar as possible from the complement, while having high similarity within the cluster, is called HNC (Hochbaum's Normalized Cut). An extensive empirical study demonstrates that incorporating pairwise similarities improves accuracy of classification and clustering. Another experimental study that compared the performance of HNC to that of the spectral technique, for imaging instances, demonstrates that in practice HNC's performance dominates the performance of the spectral technique. To address the quadratic rate of growth in the size of the data with the use of similarities we employ a method called "sparse computation" which enables the scalability of similarity-based algorithms to very large-scale data sets while maintaining high levels of accuracy. Several applications of HNC will be presented, including medical imaging; image segmentation tasks and the recent use of HNC for cell identification in neuroscience datasets.

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IP4

Diffusion-Based Methods for Biological Network Analysis

Algorithms for machine learning tasks fall most often in the realm of AI or continuous optimization of intractable problems. We present combinatorial algorithms for machine learning, data mining, and image segmentation that, unlike the majority of existing machine learning methods, utilize pairwise similarities. These algorithms are efficient and reduce the classification problem to a network flow problem on a graph. One of these algorithms addresses the problem of finding a cluster that is as dissimilar as possible from the complement, while having high similarity within the cluster, is called HNC (Hochbaum's Normalized Cut). An extensive empirical study demonstrates that incorporating pairwise similarities improves accuracy of classification and clustering. Another experimental study that compared the performance of HNC to that of the spectral technique, for imaging instances, demonstrates that in practice HNC's performance dominates the performance of the spectral technique. To address the quadratic rate of growth in the size of the data with the use of similarities we employ a method called "sparse computation" which enables the scalability of similarity-based algorithms to very large-scale data sets while maintaining high levels of accuracy. Several applications of HNC will be presented, including medical imaging; image segmentation tasks and the recent use of HNC for cell identification in neuroscience datasets.

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IP5

Scaling up Network Centrality Computations

Network science methodology is increasingly applied to a large variety of real-world phenomena, often leading to big network data sets. Thus, networks (or graphs) with millions or billions of edges are more and more common. To process and analyze these data, we need appropriate graph processing systems and fast algorithms. Yet, many analysis algorithms were pioneered on small networks when speed was not the highest concern. Developing an analysis toolkit for large-scale networks thus often requires faster variants, both from an algorithmic and an implementation perspective. In this talk, we focus on computational aspects of vertex centrality measures, as encountered in our work on the NetworKit toolkit. Such measures indicate the (relative) importance of a vertex based on its position in the network. We describe several common measures, some based on shortest paths, others on algebraic concepts. Our focus is on techniques to compute corresponding vertex rankings efficiently on large networks - in particular via approximation and parallelism. Finally, we sketch families of hard optimization problems in the centrality context and point to appropriate solution methods as well as open problems.

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JP1

Towards Scalable and Practical Real-Time Computational Epidemiology

Infectious diseases cause more than 10 million deaths a year worldwide. Globalization, urbanization, climate change, and ecological pressures increase the risk and impact of future pandemics. The ongoing COVID-19 pandemic has exemplified many of these issues. The social, economic, and health impact of the COVID-19 pandemic has been immense and will continue to be felt for decades to come. AI, data science, and scalable computation can play a multifaceted role in reorganizing, augmenting and supporting global real-time epidemic science and the rapid translation to practical public health systems. Since February 2020, our group has been providing local, state, and federal authorities continuous modeling and analytics support to contain the COVID-19 pandemic. The talk will give an overview of the state of the art in real-time computational epidemiology. Then using COVID-19 as an exemplar, we will describe how scalable computing, AI and data science can play an important role in advancing real-time epidemic science. Computational challenges , combinatorial problems and directions for future research will be discussed.

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CP1

Jacobian Sparsity Detection using Bloom Filters

Determining Jacobian sparsity structure is an important step in the efficient computation of sparse Jacobians. We introduce a new method for determining Jacobian sparsity patterns by combining bit vector probing with Bloom filters. We further refine Bloom filter probing by combining it with hierarchical probing to yield a highly effective strategy for Jacobian sparsity pattern determination.

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CP1

Queues with Small Advice

Motivated by recent work on scheduling with predicted job sizes, we consider the performance of scheduling algorithms with minimal advice, namely a single bit. The analysis of such schemes, besides demonstrating the power of very limited advice, is quite natural. In the prediction setting, one bit of advice can be used to model a simple prediction as to whether a job is “large’ or “small’; that is, whether a job is above or below a given threshold. Further, one-bit advice schemes can correspond to mechanisms that tell whether to put a job at the front or the back for the queue, a limitation which may be useful in many implementation settings. Finally, queues with a single bit of advice have a simple enough state that they can be analyzed in the limiting mean-field analysis framework for the power of two choices. Our work follows in the path of recent work by showing that even small amounts of even possibly inaccurate information can greatly improve scheduling performance.

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CP1

The Quantile Matching Problem and Point Cloud Registration

One of the fundamental problems in computer vision is the matching of two point clouds. For the case when the two point clouds do not match exactly we introduce a new approach based on quantile matching using curvature information. We define the quantile matching problem on a bipartite graph, the two parts of which represent two point clouds. The goal is to achieve an optimal registration of a point cloud with another point cloud. The problem is posed as the problem of computing a (perfect when possible) matching, which maximizes the α-quantile of affinity weights between the nodes of the graph. We prove that the problem is polynomially solvable in bipartite and non-bipartite graphs. Numerical illustrations are given. Implementations of the proposed algorithms in Python are described along with computational results with synthetic as well as real data from an optical coherence tomography application.

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CP1

General Discussion and Q&A

General discussion.

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CP2

A Parallel Approximation Algorithm for Maximizing Submodular b-matching

We design new serial and parallel approximation algorithms for computing a maximum weight b-matching in an edge-weighted graph with a submodular objective function. This problem is NP-hard; the new algorithms have approximation ratio 1/3 and are relaxations of the Greedy algorithm that rely only on local information in the graph, making them parallelizable. We have designed and implemented Local Lazy Greedy algorithms for both serial and parallel computers. We have applied the approximate submodular b-matching algorithm to assign tasks to processors in the computation of Fock matrices in quantum chemistry on parallel computers, in order to balance the computational load on the processors and bound the number of messages that a processor sends. We show that an assignment of tasks to processors here provides a four fold speedup over the currently used assignment in the NWChemEx software on 8000 processors on the Summit supercomputer at Oak Ridge National Lab.

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CP2

Fully-Dynamic Weighted Matching Approximation in Practice

Finding large or heavy matchings in graphs is a ubiquitous combinatorial optimization problem. In this paper, we engineer the first non-trivial implementations for approximating the dynamic weighted matching problem. Our first algorithm is based on random walks/paths combined with dynamic programming. The second algorithm has been introduced by Stubbs and Williams without an implementation. Roughly speaking, their algorithm uses dynamic unweighted matching algorithms as a subroutine (within a multilevel approach); this allows us to use previous work on dynamic unweighted matching algorithms as a black box in order to obtain a fully-dynamic weighted matching algorithm. We empirically study the algorithms on an extensive set of dynamic instances and compare them with optimal weighted matchings. Our experiments show that the random walk algorithm typically fares much better than Stubbs/Williams (regarding the time/quality tradeoff), and its results are often not far from the optimum.

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CP2

Using Predicted Weights for Ad Delivery

We study the performance of a proportional weights algorithm for online capacitated bipartite matching modeling the delivery of impression ads. The algorithm uses predictions on the advertiser nodes to match arriving impression nodes fractionally in proportion to the weights of its neighbors. This paper gives a thorough empirical study of the performance of the algorithm on a data-set of ad impressions from Yahoo! and shows its superior performance compared to natural baselines such as a greedy water-filling algorithm and the ranking algorithm. The proportional weights algorithm has recently received interest in the theoretical literature where it was shown to have strong guarantees in the beyond the worst-case model of algorithms augmented with predictions. We extend these results to the case where the advertisers capacities are no longer stationary over time. Additionally, we show the algorithm has near optimal performance in the random-order arrival model when the number of impressions and the optimal matching are sufficiently large.

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CP3

A Metric on Directed Graphs and Markov Chains based on Hitting Probabilities

The shortest-path, commute time, and diffusion distances on undirected graphs have been widely employed in applications such as dimensionality reduction, link prediction, and trip planning. Increasingly, there is interest in using asymmetric structure of data derived from Markov chains and directed graphs, but few metrics are specifically adapted to this task. We introduce a metric on the state space of any ergodic, finite-state, time-homogeneous Markov chain and, in particular, on any Markov chain derived from a directed graph. Our construction is based on hitting probabilities, with nearness in the metric space related to the transfer of random walkers from one node to another at stationarity. Notably, our metric is insensitive to shortest and average walk distances, thus giving new information compared to existing metrics. We use possible degeneracies in the metric to develop an interesting structural theory of directed graphs and explore a related quotienting procedure. Our metric can be computed in $O(n^3)$ time, where n is the number of states, and in examples we scale up to $n = 10,000$ nodes and $\approx 38M$ edges on a desktop computer. In several examples, we explore the nature of the metric, compare it to alternative methods, and demonstrate its utility for weak recovery of community structure in dense graphs, visualization, structure recovering, dynamics exploration, and multiscale cluster detection.

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CP3

Non-Monotone Adaptive Submodular Meta-Learning

The core idea of meta-learning is to leverage prior experience to design solutions that can be quickly adapted to new, unseen tasks. Most of existing studies consider the case where the feasible parameter space is continuous. Recently, [**?**] develops the framework of a discrete variant of meta-learning, called submodular meta-learning, and they treat each task as a discrete optimization problem, i.e., they intend to select a group of items that maximizes the average expected utility of all tasks. Motivated by their framework, we consider the submodular meta-learning problem under the adaptive setting. In particular, we assume that each item has a random state, which is drawn from some known prior distribution. One must select an item before observing its realized state. Given a task, the utility function is defined over items and states. Our goal is to adaptively select a group items, each selection is based on the feedback from the past, to maximize the average expected utility of all tasks. Following the framework of standard meta-learning, we propose an effective policy that is composed of two phases: We first pre-compute an initial set of items, called initial solution set, based on previously visited tasks, then, once a new task is revealed, we add more items to the initial solution set to complete the selection process. We show that our policy achieves a 1/32 approximation ratio if the utility function of each task is adaptive submodular.

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CP3

Local Hyper-Flow Diffusion

Recently, hypergraphs attracted a lot of attention due to their ability to capture complex relations among entities. The insurgence of hypergraphs has resulted in data of increasing size and complexity that exhibit interesting small-scale and local structure, e.g., small-scale communities and localized node-ranking around a given set of seed nodes. Popular and principled ways to capture the local structure are the local hypergraph clustering problem and the related seed set expansion problem. In this work, we propose the first local diffusion method that achieves edge-size-independent quadratic approximation error for the problem of local hypergraph clustering, while applying to a substantially richer class of higher-order relations with only a submodularity assumption. Our method is based on a primal-dual optimization formulation where the primal problem has a natural network flow interpretation, and the dual problem has a cut-based interpretation using the ℓ_2-norm penalty on associated cut-costs. We demonstrate the new technique is significantly better than state-of-the-art methods on both synthetic and real-world data.

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CP3

Binary Level-Set Method for Variational Implicit Solvation Model

The Variational Implicit Solvent Model (VISM) is a theoretical and computational tool to study biomolecular systems with complex topology. Central in VISM is an effective free-energy of all possible interfaces separating solutes (e.g., proteins) from solvent (e.g., water). Such a functional can be minimized numerically by a level-set method to determine the stable equilibrium conformations and solvation free energies. However, the PDE-based approach is time-consuming. We developed a discrete formulation of the problem using the binary level set method. The interface is approximated by a binary level set function that takes value ± 1 on the solute/solvent region. The VISM energy can be minimized by iteratively "flipping' the binary level set function. The new method is fast enough to be coupled with the Monte Carlo method for biomolecular simulations. We also show that with the discrete formulation, the VISM energy functional can be globally minimized by min-cut max-flow algorithms.

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CP4

Shared-Memory Implementation of the Karp-Sipser Kernelization Process

We investigate the parallelization of the Karp-Sipser kernelization technique, which constitutes the central part of the well known Karp-Sipser heuristic for the maximum cardinality matching problem. The technique reduces a given problem instance to a smaller but equivalent one, by a series of two operations: vertex removal, and merging/unifying two vertices. The operation of merging two vertices poses the principal challenge in parallelizing the technique. We describe an algorithm that minimizes the need for synchronization and present an efficient shared-memory parallel implementation. Using extensive experiments on a variety of multicore CPUs, we show that our implementation scales well up to 32 cores on one socket.

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CP4

On the Difference Between Search Space Size and Query Complexity in Contraction Hierarchies

In this paper we present results that underline the significant difference between the size of node search space size and the query complexity in Contraction Hierarchies. Under different input models, node search spaces were proven to be sublinear. In this paper we prove for the same settings that edge search spaces are not sublinear. Our results make clear, that only analyzing the number of processed nodes during a CH query does not suffice for a thorough understanding of the CH query complexity. A broader definition of the search space that takes edges into account appears to be necessary.

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CP4

Improving Tug-of-War Sketch using Control-Variates Method

Computing space-efficient summary, or *a.k.a. sketches*, of large data, is a central problem in the streaming algorithm. Such sketches are used to answer *post-hoc* queries in several data analytics tasks. The algorithm for computing sketches typically requires to be fast, accurate, and space-efficient. In this work, we focus on the problem of computing frequency moments of a data stream and computing the inner product of the frequency vectors corresponding to a pair of data streams. The seminal work of Alon, Matias, and Szegedy, *a.k.a. Tug-of-war* sketch gives a randomized sublinear space (and linear time) algorithm for these problems. However, the variance of the estimates given by the Tug-of-war sketch typically tends to be large. In this work, we focus on minimizing the variance of these estimates using the techniques from the classical Control-Variate method, which is primarily known for variance reduction in Monte-Carlo simulations. As a consequence, we are able to obtain significant variance reduction, at the cost of a little computational overhead. We present a theoretical analysis of our proposal and complement it with supporting experiments on synthetic as well as real-world datasets.

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CP5

Fairmandering: A Column Generation Heuristic for Fairness-Optimized Political Districting

The American winner-take-all congressional district system empowers politicians to engineer electoral outcomes by manipulating district boundaries. Existing computational solutions mostly focus on drawing unbiased maps by ignoring political and demographic input, and instead simply optimize for compactness. We claim that this is a flawed approach because compactness and fairness are orthogonal qualities, and introduce a scalable two-stage method to explicitly optimize for arbitrary piecewise-linear definitions of fairness. The first stage is a randomized divide-and-conquer column generation heuristic which produces an exponential number of distinct district plans by exploiting the compositional structure of graph partitioning problems. This district ensemble forms the input to a master selection problem to choose the districts to include in the final plan. Our decoupled design allows for unprecedented flexibility in defining fairness-aligned objective functions. The pipeline is arbitrarily parallelizable, is flexible to support additional redistricting constraints, and can be applied to a wide array of other regionalization problems. In the largest ever ensemble study of congressional districts, we use our method to understand the range of possible expected outcomes and the implications of this range on potential definitions of fairness.

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CP5

Faster Parallel Multiterminal Cuts

We give an improved branch-and-bound solver for the multiterminal cut problem, based on the recent work of Henzinger et al. We contribute new, highly effective data reduction rules to transform the graph into a smaller equivalent instance. In addition, we present a local search algorithm that can significantly improve a given solution to the multiterminal cut problem. Our exact algorithm is able to give exact solutions to more and harder problems compared to the state-of-the-art algorithm by Henzinger et al.; and give better solutions for more than two third of the problems that are too large to be solved to optimality. Additionally, we give an inexact heuristic algorithm that computes high-quality solutions for very hard instances in reasonable time.

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CP5

Augmented Sparsifiers for Generalized Hypergraph Cuts

A number of recent advances in hypergraph clustering and related higher-order machine learning tasks rely on minimizing generalized hypergraph cut functions. These assign different cut penalties for different ways of partitioning the nodes of a hyperedge. We introduce new techniques for approximately solving generalized hypergraph cut problems by reducing a hypergraph to a sparse directed graph on an augmented set of nodes. We show that this can be accomplished by finding piecewise linear approximations to certain concave functions representing cut penalties. In addition to producing faster algorithms for the minimum hypergraph s-t cut problem, our sparsification technique leads to improved sparsifiers for graphs constructed from co-occurrence data, as well as faster approximation algorithms for minimizing certain classes of decomposable submodular functions.

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CP6

Parameterized Algorithms for Identifying Gene Co-Expression Modules via Weighted Clique Decomposition

We present a new combinatorial model for identifying regulatory modules in gene co-expression data using a decomposition into weighted cliques. To capture complex interaction effects, we generalize the previously-studied weighted edge clique partition problem. As a first step, we restrict ourselves to the noise-free setting, and show that the problem is fixed parameter tractable when parameterized by the number of modules (cliques). We present two new algorithms for finding these decompositions, using linear programming and integer partitioning to determine the clique weights. Further, we implement these algorithms in Python and test them on a biologically-inspired synthetic corpus generated using real-world data from transcription factors and a latent variable analysis of co-expression in varying cell types.

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CP6

BELLA: Berkeley Efficient Long-Read to Long-Read Aligner and Overlapper

Recent advances in long-read sequencing allow characterization of genome structure and its variation within and between species at a resolution not previously possible. Detecting overlap between reads is an essential component of many long-read genome pipelines, such as de novo genome assembly. Longer reads simplify genome assembly and improve reconstruction contiguity, but current long-read technologies are associated with moderate to high error rates. Here we present BELLA, a novel algorithm for overlap detection and alignment using sparse matrix-matrix multiplication. Furthermore, we present a probabilistic model that demonstrates the feasibility of using k-mers for overlap detection and shows its flexibility when applied to different k-mer selection strategies. Based on such a model, we introduce a notion of reliable k-mers. Combining reliable k-mers with our binning mechanism increases the computational efficiency and accuracy of our algorithm. Finally, we introduce a new method based on Chernoff bounds to separate true overlaps from false positives using a combination of alignment techniques and probabilistic modeling. Our goal is to maximize the balance of precision and recall. BELLA is among the best F1 scores and exhibits performance stability than competing software often lacks. BELLA's F1 score is consistently within 1.7% of the top performer. BELLA improves the de novo assembly quality on synthetic data when coupled with the Miniasm assembler.

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CP6

Elruna : Elimination Rule-Based Network Alignment

In this paper, we propose ELRUNA (elimination rule-based network alignment), a novel network alignment algorithm that relies exclusively on the underlying graph structure. Under the guidance of the elimination rules that we defined, ELRUNA computes the similarity between a pair of cross-network vertices iteratively by accumulating the similarities between their selected neighbors. The resulting cross-network similarity matrix is then used to infer a permutation matrix that encodes the final alignment of cross-network vertices. In addition to the novel alignment algorithm, we improve the performance of local search, a commonly used postprocessing step for solving the network alignment problem, by introducing a novel selection method RAWSEM (random walk-based selection method) based on the propagation of vertices mismatching across the networks. The key idea is to pass on the initial levels of mismatching of vertices throughout the entire network in a random-walk fashion. Through extensive numerical experiments on real networks, we demonstrate that ELRUNA significantly outperforms the state-of-the-art alignment methods in terms of alignment accuracy under lower or comparable running time. Moreover, ELRUNA is robust to network perturbations such that it can maintain a close to optimal objective value under a high level of noise added to the original networks. Finally, the proposed RAWSEM can further improve the alignment quality compared with the naive local search method.

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CP7

Sphynx: A Parallel Multi-GPU Graph Partitioner

Graph partitioning has been an important tool to partition the work among several processors to minimize the communication cost and balance the workload. While accelerator-based supercomputers are emerging to be the standard, the use of graph partitioning becomes even more important as applications are rapidly moving to these architectures. However, there is no distributed-memory parallel, multi-GPU graph partitioner available for applications. We developed a spectral graph partitioner, Sphynx, using the portable, accelerator-friendly stack of the Trilinos framework. In Sphynx, we allow using different preconditioners and exploit their unique advantages. We use Sphynx to systematically evaluate the various algorithmic choices in spectral partitioning with a focus on the GPU performance. We perform those evaluations on two distinct classes of graphs: regular (such as meshes, matrices from finite element methods) and irregular (such as social networks and web graphs), and show that different settings and preconditioners are needed for these graph classes. The experimental results on the Summit supercomputer show that Sphynx is the fastest alternative on irregular graphs in an application-friendly setting and obtains a partitioning quality close to ParMETIS on regular graphs. Sphynx provides a good and robust partitioning method across a wide range of graphs for applications looking for a GPU-based partitioner.

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CP7

A Message-Driven, Multi-GPU Parallel Sparse Triangular Solver

Sparse triangular solve is used in conjunction with Sparse LU for solving sparse linear systems, either as a direct solver or as a preconditioner. As GPUs have become first-class compute citizens, designing an efficient and scalable SpTRSV on multi-GPU HPC systems is imperative. In this paper, we leverage the advantage of GPU-initiated data transfers of NVSHMEM to implement and evaluate a Multi-GPU SpTRSV. We create a novel producer-consumer paradigm to manage the computation and communication in SpTRSV and implement it using two CUDA streams. Our multi-GPU SpTRSV implementation using CUDA streams achieves up to a 3.7× speedup when using up to eighteen GPUs (three nodes) relative to our implementation on a single GPU, and up to 6.1× compared to cusparse_csrsv2() with a scale from single GPU to eighteen GPUs. To further explain the observed performance and explore the key features of matrices to estimate the potential performance benefits when using multi-GPU, we extend the critical path model of SpTRSV to GPUs. We demonstrate the ability of our performance model to understand various aspects of performance and performance bottlenecks on multi-GPU and motivate code optimizations.

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CP7

Parallel Clique Counting and Peeling Algorithms

We present a new parallel algorithm for k-clique counting/listing that has polylogarithmic span (parallel time) and is work-efficient (matches the work of the best sequential algorithm) for sparse graphs. Our algorithm is based on computing low out-degree orientations, which we present new work-efficient parallel algorithms for. We also present new parallel algorithms for approximate clique counts using graph sparsification. Finally, we design two new parallel work-efficient algorithms for approximating the k-clique densest subgraph, the first of which is a $1/k$-approximation and the second of which is a $1/(k(1+\epsilon))$-approximation and has polylogarithmic span. Our first algorithm does not have polylogarithmic span, but we prove that it solves a P-complete problem. In addition to the theoretical results, we implement the algorithms and propose optimizations to improve their practical performance. On a 30-core machine with two-way hyper-threading, our algorithms achieve 13.23–38.99x and 1.19–13.76x self-relative parallel speedup for k-clique counting and k-clique densest subgraph, respectively. Compared to the state-of-the-art parallel k-clique counting algorithms, we achieve up to 9.88x speedup, and compared to existing implementations of k-clique densest subgraph, we achieve up to 11.83x speedup. We are able to compute the 4-clique counts on the largest publicly-available graph with over two hundred billion edges for the first time.

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CP8

A Dynamic Program for Computing the Joint Cumulative Distribution Function of Order Statistics

We consider the problem of computing the joint cumulative distribution function of d select order statistics of $n \geq d$ independent random variables representing $m \leq n$ distinct populations. We present an efficient dynamic programming algorithm for this problem that is polynomial in both d and n, though exponential in m, hence most practical when $m \ll n$. Previously, the fastest known algorithms were exponential in d, and either exponential in m or exponential in n, as well. Like others before us, we reduce the problem to a combinatorial one of tossing balls into bins, and then we calculate the probability of satisfying various bin conditions: i.e., of sufficiently many balls landing in bins. The key observation that leads to such a significant speedup is that one need not keep track of the exact configurations of balls in bins to determine if the requisite bin conditions are satisfied. Instead, the relevant information can be compressed by merging configurations that satisfy the same bin conditions.

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CP8

Optimal Portfolio Execution in a Regime-Switching Market with Non-Linear Impact Costs: Combining Dynamic Program and Neural Network

Optimal execution of a portfolio have been a challenging problem for institutional investors. Traders face the trade-off between average trading price and uncertainty. Traditional methods suffer from the curse of dimensionality, and easily become intractable when multiple assets are considered. Here, we consider a set of discrete chunks, and propose a four-step numerical framework for the optimal portfolio execution problem where multiple market regimes exist, with the underlying regime switching based on a Markov process. The market impact costs are modelled with a temporary part and a permanent part, where the former affects only the current trade while the latter persists. Our approach accepts impact cost functions in generic forms, and provides robust strategies for both CRRA (constant relative risk aversion) and mean-variance objective functions.

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CP9

Efficient Signed Backward Substitution for Piecewise Affine Functions via Path Problems in a Directed Acyclic Graph

We introduce an efficient signed backward substitution for a highly-structured system. More precisely, the problem is to find a vector u of dimension s that solves the system of piecewise affine equations $u = c + L|u|$, where L is a strictly lower left triangular $s \times s$ matrix, c denotes a given vector of dimension s, and the notation $|\cdot|$ indicates the component-wise absolute value of a vector. The novel approach is based on a Neumann series reformulation and attempts to exploit a high degree of parallelism. We provide an analysis of its parallel run-time and show that it is suited for large, sparse systems whose triangular matrix has a small switching depth. The general idea behind this approach which is also used in the convergence proof is based on modelling the switching depth by a graph theoretic model. The key observation is that the computation of the switching depth corresponds to a single-pair shortest path problem in a directed acyclic graph. The proposed method is implemented and numerically evaluated using several examples whose problem structures are representative of various applications in scientific computing.

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CP9

Limitations of Chung-Lu Random Graph Generation

Random graph models play a central role in the study of social networks and in broader network analysis. The

Chung-Lu model, which connects nodes v_i, v_j based on their expected degrees w_i,w_j according to the attachment probabilities $\frac{w_i w_j}{\sum w_k}$, is of particular interest. It is widely used to generate null-graph models with expected degree sequences. In addition, these attachment probabilities implicitly define network measures such as modularity. Despite its popularity, practical methods for generating instances of Chung-Lu model-based graphs do relatively poor jobs in terms of accurately realizing many degree sequences. We perform a theoretical analysis of the Chung-Lu random graph model in order to understand this discrepancy. We approximate the output of the Chung-Lu random graph model with a linear system and use properties of this system to predict distribution errors. We provide bounds on the maximum proportion of nodes with a given degree that can be reliably produced by the model for both general and non-increasing distributions. We additionally provide an explicit inverse of our linear system and in cases where the inverse is non-negative, we introduce a simple method for improving the accuracy of Chung-Lu graph generation. Our analysis serves as an analytic tool for determining the accuracy of Chung-Lu random graph generation as well as correcting errors under certain conditions.

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CP9

Multidimensional Included and Excluded Sums

This paper presents algorithms for the included-sums and excluded-sums problems used by scientific computing applications such as the fast multipole method. These problems are defined in terms of a d-dimensional array of N elements and a binary associative operator $\oplus$ on the elements. The included-sum problem requires that the elements within overlapping boxes cornered at each element within the array be reduced using $\oplus$. The excluded-sum problem reduces the elements outside each box. The weak versions of these problems assume that the operator has an inverse, whereas the strong versions do not require this assumption. In addition to studying existing algorithms to solve these problems, we introduce three new algorithms. The bidirectional box-sum (BDBS) algorithm solves the strong included-sums problem in $\Theta(dN)$ time, asymptotically beating the classical summed-area table (SAT) algorithm, which runs in $\Theta(2^d N)$ and which only solves the weak version of the problem. Empirically, the BDBS algorithm outperforms the SAT algorithm in higher dimensions by up to 17.1×. The box-complement algorithm can solve the strong excluded-sums problem in $\Theta(dN)$ time, asymptotically beating the state-of-the-art "corners' algorithm by Demaine *et al.*, which runs in $\Omega(2^d N)$ time. In 3 dimensions the box-complement algorithm empirically outperforms the corners algorithm by about 1.4× given similar amounts of space.

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CP10

RCHOL: Randomized Cholesky Factorization for Solving Sdd Linear Systems

We introduce a randomized algorithm, namely RCHOL, to construct an approximate Cholesky factorization for a given Laplacian matrix (a.k.a., graph Laplacian). The exact Cholesky factorization for the matrix introduces a clique in the associated graph after eliminating every row/column. By randomization, RCHOL keeps a sparse subset of the edges in the clique using a random sampling developed by Spielman and Kyng. We prove RCHOL is breakdown-free and apply it to solving large sparse linear systems with symmetric diagonally dominant matrices. In addition, we parallelize RCHOL based on the nested dissection ordering for shared-memory machines. Numerical experiments demonstrated the robustness and the scalability of RCHOL. For example, our parallel code scaled up to 64 threads on a single node for solving the 3D Poisson equation, discretized with the 7-point stencil on a $1024 \times 1024 \times 1024$ grid, or one billion unknowns.

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CP10

Algorithmic Techniques for Finding Resistance Distances on Structured Graphs with an Application to Linear 2-Trees

The resistance distance (occasionally referred to as the effective resistance) of a graph is a measure that quantifies its structural properties. Resistance distance in graphs has played a prominent role not only in circuit theory and chemistry, but also in combinatorial matrix theory and spectral graph theory. Moreover, resistance distance has been used in applied settings to sparsify a graphs while maintaining spectral properties, in the field of distributed control and estimation, and as a tool for link prediction in networks. The first half of the presentation will focus on common methods of determining the resistance distance in graphs and provide examples of these methods. In particular, we will discuss the the combinatorial Laplacian, electric circuit transformations, recursive techniques and spanning two forests. With each of these techniques we will include informative examples, as well as potential applications. In addition to surveying methods for calculating resistance distance, we will also discuss some results concerning resistance distance on the family of graphs known as linear 2trees. Finally we will close the presentation with several interesting open conjectures involving resistance distance.

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CP10

General Discussion and Q&A

General Discussion.

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CP10

Efficient Parallel Sparse Symmetric Tucker Decomposition for High-Order Tensors

Tensor based methods are receiving renewed attention in recent years due to their prevalence in diverse real-world applications. There is considerable literature on tensor representations and algorithms for tensor decompositions, both for dense and sparse tensors. Many applications in hypergraph analytics, machine learning, psychometry, and signal processing result in tensors that are both sparse and symmetric, making it an important class for further study. Similar to the critical Tensor Times Matrix chain operation (TTMc) in general sparse tensors, the Sparse Symmetric Tensor Times Same Matrix chain (S^3TTMc) operation is compute and memory intensive due to high tensor order and the associated factorial explosion in the number of non-zeros. In this work, we present a novel compressed storage format, CSS, for sparse symmetric tensors, along with an efficient parallel algorithm for the S^3TTMc operation. We theoretically establish that S^3TTMc on CSS achieves a better memory vs. run-time trade-off compared to state-of-the-art implementations. We demonstrate experimental findings that confirm these results and achieve up to 2.9× speedup on synthetic and real datasets.

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CP11

The Traveling Firefighter Problem

We introduce the routing problem, L_p-TSP, for which the input includes a set of destinations, the origin, along with the underlying distances. The objective is to schedule a traveler, of unit speed, to minimize the Minkowski p-norm of the consequent vector of visit/service times. For $p=\infty$ the problem becomes a path variant of the Traveling Salesman Problem and for $p=1$ it defines the Traveling Repairman Problem, both at the center of classical combinatorial optimization. L_p-TSP can be formulated as a convex mixed-integer program and enables a smooth interpolation between path-TSP and TRP, corresponding to optimal routes from the perspective of a server vs. the clients, respectively. p can affect fairness or efficiency of the solution. Case $p=2$ models the scenario when the cost/damage due to delay in service is quadratic in time, which we term as the Traveling Firefighter Problem and provide a 5.65 approximation for it, on general metrics. We also provide a reduction of L_p-TSP to segmented-TSP, resulting PTAS for the Euclidean and tree metrics, for any p. We further study all-norm-TSP, in which the objective is to find a route that is near optimal concerning the minimization of any norm of the visit times. We improve the competitive/approximation bound for this problem to 8, for general metrics, and introduce a first impossibility bound. We leave open several interesting directions to further develop this line of research.

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CP11

Search and Evacuation with a Near Majority of Faulty Agents

There are $n \geq 3$ unit speed mobile agents placed at the origin of the infinite line. In as little time as possible, the agents must find and evacuate from an exit placed at an initially unknown location on the line. The agents can communicate in the wireless mode in order to facilitate the evacuation (i.e. by announcing the target's location when it is found). However, among the agents are a subset of at most f crash faulty agents who may fail to announce the target when they visit its location. In this paper we study this aforementioned problem for the specific case that $n=2f+1$. We introduce a novel type of search algorithm and analyze its competitive ratio – the supremum, over all possible target locations, of the ratio of the time the agents take to evacuate divided by the initial distance between the agents and the target. In particular, we demonstrate that the competitive ratio of evacuation is at most 7.437011 for $(n,f)=(3,1)$; at most 7.253767 for $(n,f)=(5,2)$ and $(7,3)$; and at most 7.147026 for $(n,f)=(9,4)$. For larger values of $n=2f+1$ we prove an asymptotic upper bound of $4+2\sqrt{2}$. We also adapt our evacuation algorithm for $(n,f)=(3,1)$ to the problem of search by three agents with one byzantine fault, i.e. the faulty agent may also lie about finding the target. In doing so we improve the best known upper bound on this search problem from 8.653055 to 7.437011.

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CP11

On the Request-Trip-Vehicle Assignment Problem

The request-trip-vehicle assignment problem is at the heart of a popular decomposition strategy for online vehicle routing. In this framework, assignments are done in batches in order to exploit any shareability among vehicles and incoming travel requests. We study a natural ILP formulation and its LP relaxation. Our main result is an LP-based randomized rounding algorithm that, whenever the instance is feasible, leverages mild assumptions to return an assignment whose: i) expected cost is at most that of an optimal solution, and ii) expected fraction of unassigned requests is at most $1/e$. If trip-vehicle assignment costs are α-approximate, we pay an additional factor of α in the expected cost. We can relax the feasibility requirement by considering the penalty version of the problem, in which a penalty is paid for each unassigned request. We find that, whenever a request is repeatedly unassigned after a number of rounds, with high probability it is so in accordance with the sequence of LP solutions and not because of a rounding error. We additionally introduce a deterministic rounding heuristic inspired by our randomized technique. Our computational experiments show that our rounding algorithms achieve a performance similar to that of the ILP at a reduced computation time, far improving on our theoretical guarantee. The reason for this is that, although this assignment problem is hard in theory, its natural LP relaxation tends to be very tight in practice.

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MS0

Performance Analysis of HPC Applications

We present a method for performance analysis of distributed HPC applications. The method is based on representing application trace as a DAG of communication calls, function calls and kernel calls. For applications running on up to 16 GPUs the application graph normally has several millions of nodes and arcs. The application graph allows to estimate concurrency across kernels, overlap of computations and communications, overhead due to synchronizations. The application graph can be mapped on future architectures to predict performance of the application. We will list a few problems that impede application analysis: detecting loop nests (graph FFT), identifying irreducible core of the application graph, calculating the skeletones, deleting shortcuts and DAG visualizations.

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MS0

What's left in dictionary design?

The last two decades have seen phenomenal advances in the design of external-memory dictionaries, largely driven by the needs of internet-scale big-data companies, such as Google and Facebook. This talk will outline a few research questions for where to go next in the design of dictionary data structures. Surprisingly, there may still be an order-of-magnitude of performance on the table, but we're probably going to have to start looking at the actual data in order to grab it.

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MS0

Next Generation of Parallel and Distributed Graph Mining Algorithms: Theory and Practice

We present two approaches to scaling up graph algorithms in theory and practice. First, we show how to take advantage of a distributed hash table to obtain a more powerful model of distributed computation [SPAA'19]. In this model, we give new algorithms for fundamental graph problems, such as connected components, minimum spanning tree, maximum matching and maximal independent set, which use much fewer rounds in theory and work up to 7x faster in practice [VLDB'20]. Second, we present our single-machine algorithms capable of clustering 1B edge graphs in under 2 minutes, which uses shared-memory parallelism. To do so, we apply GBBS framework, and also present fast parallel algorithms for a range of graph clustering problems, e.g., linear-time algorithms with polylogarithmic depth for min-size clustering, and hierarchical clustering [ICML'21,Arxiv].

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MS0

Mixed Integer Programming - A Confluence of Algorithms

Mixed Integer Programming (MIP) is a powerful technology that is used in a variety of applications. While people often ask what algorithm is used to solve MIP models, the reality is that a modern MIP solver combines algorithms from a wide range of domains, including linear algebra, number theory, polyhedral mathematics, numerical analysis, graph theory, parallel computing, group theory, ... The underlying MIP problem is NP-hard, so the best we can expect from each ingredient is to chip away at some part of the imposing whole. We'll talk about some of the techniques that go into a modern MIP solver, and discuss the extent to which each is able to manage the task put in front of it.

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MT0

An Introduction to Combinatorial Scientific Computing

Graph algorithms have played an important role in numerical methods since at least 1961 when Parter noted that graphs could be used to describe the structure of sparse matrix algorithms. Through the intervening decades, graphs have been used to encode a wide variety of concepts in scientific computing and have played key roles in sparse factorizations, parallel algorithms, algorithmic differentiation, mesh generation and many other problems. In the early 2000s, researchers in this field coalesced around the name Combinatorial Scientific Computing (CSC). A series of SIAM Workshops on CSC has now been folded into the new ACDA Conference. This minitutorial will provide an accessible introduction to CSC with a focus on three illustrative research topics: (i) applications of graph matching for entity pairing, (ii) large-scale graph partitioning for load balancing, and (iii) graph models in algorithmic differentiation for computing exact derivatives of computer-generated functions. Through these exemplar problems we will touch on some of the recurring elements of CSC including: Graph abstractions in numerical algorithms Practical approximation algorithms for expensive graph operations Empirical performance studies Performance on modern and emerging computer architectures Connections between scientific computing and data mining

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MT0

Combinatorial Frontiers in Computational Biology

There are numerous subfields of computational biology and bioinformatics where important mathematical questions arise that require a combinatorics or graph theory toolbox. This tutorial will introduce some biological problems that are ripe for collaboration opportunities with the ACDA community. We will provide a high-level overview of the landscape and then focus on two emerging "hot topic" areas protein-protein interaction networks and single cell sketching. For the first topic, we will provide an overview of network science methods in protein-protein interaction networks, which will set the stage for the ACDA21 plenary talk by Prof. Lenore Cowen. The second topic area will be on the challenge of representing, denoising, and ultimately sketching single cell data. This work includes applications of spectral graph theory and manifold learning to denoise and model cellular systems faithfully for predictive insight. This mini-tutorial aims to introduce a set of biologically-important yet mathematically deep problems in an accessible way to applied mathematicians with little prior engagement with biology.

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PP0

1 - Families of Optimization Problems Related to Network Centrality

Networks (or graphs) are widely used to model relationships in numerous real-world applications, and network analysis aims to unveil hidden information or patterns in the structure of those networks. Centrality measures indicate the importance of a vertex (or edge) in the network and are widely used for network analysis. Numerous measures exist, some based on shortest paths, others consider paths of arbitrary lengths none is universal and appropriate for all applications. In this poster, we present our research on three families of centrality-related optimization problems: - group centrality maximization - centrality improvement - graph robustness Our solution methods are designed for specific centrality measures; yet, the generic optimization problems can be parameterized with any such measure. The resulting approximation algorithms are able to scale to much larger instances than the state of the art, while the solution quality in practice is often comparable.

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2 - Analytic Solutions to Quadratic Programs

In 2011, a fascinating paper appeared in the Journal of Portfolio Management. Its authors (Clarke, De Silva & Thorley 2011) produced an analytic expression for a minimum variance portfolio without short sales. The expression solved an important special case of a problem in optimization theory. While the formula of Clarke et al. (2011) had no rigorous proof, contained an error and had a narrow scope, it supplied a new result. Unfortunately, the focus of the authors and the journal on portfolio theory obscured this novel contribution to the field of numerical optimization generally, and quadratic programming in particular. We extend the results of Clarke et al. (2011) establishing a rigorous theoretical foundation. Specifically, we develop analytic expressions for solutions to quadratic programs constrained to a standard simplex currently only solvable numerically. Our approach uses fixed point theory to characterize the solution in a way that reveals its geometric properties. The associated fixed-point maps are discontinuous necessitating an analysis that does not rely on contraction properties. When the objective matrix has a factor structure, our fomulae also yield highly efficient algorithms. The iterates of these algorithms behave very differently from those produced by traditional numeric solvers. We analyze the complexity of our algorithms, develop a corresponding convergence theory, and benchmark them against state-of-the-art.

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PP0

3 - A Dynamic Programming Heuristic for Dense Hessian Chain Bracketing

Second derivatives of mathematical models for real-world phenomena are fundamental ingredients of a wide range of numerical simulation methods including parameter sensitivity analysis, uncertainty quantification, nonlinear optimization and model calibration. The evaluation of such Hessians often dominates the overall computational effort. Various combinatorial optimization problems can be formulated based on the highly desirable exploitation of the associativity of the chain rule of differential calculus. The fundamental HESSIAN ACCUMULATION problem aiming to minimize the number of floating-point operations required for the computation of a Hessian turns out to be NP-complete. The restriction to suitable subspaces of the exponential search space proposed in this paper ensures computational tractability while yielding improvements by factors of ten and higher over standard approaches based on second-order tangent and adjoint algorithmic differentiation. This paper focusses on bracketing of dense Hessian chain products with the aim of minimizing the total number of floating-point operations to be performed. The results from a given dynamic programming algorithm for optimized bracketing of the underlying dense Jacobian chain product are used to reduce the computational cost of the corresponding Hessian. Minimal additional algorithmic effort is required.

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4 - Parallel Nearest Neighbors in Low Dimensions with Batch Updates

We present a set of parallel algorithms for computing exact k-nearest neighbors in low dimensions. Most k-nearest neighbor algorithms in the literature use either a kd-tree or the Morton ordering of the set of points: our algorithm combines these approaches. We present a variant of our algorithm specialized for computing the k-nearest neighbor graph of an entire point set, and one for general queries. Furthermore, both of these variants support batch-dynamic insertions to the original data structure; to our knowledge, these are the first k-nearest neighbor algorithms to support batch-dynamic updates. We benchmark our algorithms against existing parallel nearest neighbor algorithms, experimenting on tree-based implementations as well as implementations based on the Morton ordering. Our experimental results show that our implementations are generally faster than all the algorithms we use to benchmark, as well as achieving 75x speedup for calculating all nearest neighbors on 144 cores. Our batch-dynamic insertions achieve 10^{-3} speedup per element for a batch of size 5 million.

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5 - Robust Problems in General Norms

We initiate study of robust combinatorial optimization problems in general norms. The contribution is as follows: - we develop a general framework based on LP formulation that is applicable to several instances of combinatorial optimization problems including shortest paths and matroid optimization, - we prove that problems falling into our framework can be solved efficiently with arbitrary small error in polynomial time for general perturbation norms, e.g., L_p-norms, - we present a more efficient instantiation of our framework in the case of L_1-norm, - we derive a possible approach how to handle multi-objective versions of robust problems. To the best of our knowledge, no framework this general has been developed before. Previous research focuses on specific problems, e.g., shortest paths, or matroid optimization, and/or is limited to specific perturbation norms, e.g., L_1.

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6 - Spectral Hypergraph Partitioning Revisited

Most state-of-the-art hypergraph partitioning algorithms follow a multilevel approach that constructs a hierarchy of coarser hypergraphs that in turn are used to drive partition refinements. These partitioners are widely accepted as the current standard, as they have proven to be quite effective. On the other hand, spectral partitioners are considered to be less effective in cut quality, and too slow to be used in industrial applications. In this work, we revisit spectral hypergraph partitioning and we demonstrate that the use of appropriate solvers eliminates the running time deficiency. In fact, spectral algorithms can compute competing solutions in a fraction of the time needed by standard partitioning algorithms, especially on larger designs. We also introduce several novel modifications in the common spectral partitioning workflow, that enhance significantly the quality of the computed solutions. We run our partitioner on FPGA benchmarks generated by an industry leader, generating solutions that are directly competitive both in runtime and quality.

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8 - A Framework for Efficient Line Graph Computation for Hypergraphs

Hypergraphs are increasingly becoming important in data science applications due to their capability for robust data representation. However, their computational complexity can be high. To reduce this complexity, lower order approximations of hypergraph to compute relevant structures are often employed. Line graphs, in particular, higher order s-line graphs for $s > 1$, of hypergraphs can be considered as a critical tool for this purpose. Such line graphs are sufficient to capture important hypergraph properties, while leveraging fine-tuned graph algorithms on the s-line graphs to approximate different hypergraph metrics. Obtaining high order s-line graphs is highly compute-intensive. In this work, we present a framework for s-line graph computations, including efficient, parallel algorithms to accelerate s-line graphs computation, and demonstrate approximately 1.4× to 9× speedup compared to a prior state of the art algorithm proposed recently. To the best of our knowledge, ours is the first framework for high order line graph computation of hypergraphs.

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7 - Theoretical Study of DenseNet Scheduling on Heterogeneous System Architecture

This paper discusses the scheduling problem for DenseNet on a heterogeneous system. DenseNet is a promising network topology for AI learning. It has extensive data dependency, so it is very challenging to schedule the tasks among processing units. Modern computing systems have heterogeneous processors for different computing needs, and communication among processors is expensive. Therefore, it is essential to scheduling the computation tasks to the suitable processors while reducing the communication among them. We show that the DenseNet scheduling problem is NP-Complete when the number of heterogeneous processors is n^2, where n is the size of the DenseNet. Nevertheless, we show that when there are only *two* heterogeneous processors, dynamic programming can schedule the DenseNet computation optimally in $O(n)$ time by a series of optimizations. This heterogeneous system model is consistent with the current computer systems, which mostly have one CPU and one GPU as the primary resources for AI computation. We also implement these algorithms and compare their timing results. The dynamic programming relies on two keen observations to improve the time complexity. First, we observe that the delay effect due to communication will not affect later tasks assigned to the same processor. Second, we observe that we can simplify the dependency by considering one task at a time in increasing time order and perform an amortized cost analysis over all tasks.

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9 - MTK: A Composable Graph Transformation System for Equation-Based Modeling

Not available

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10 - Classifying E-Commerce Product Listings using Word Co-Occurrence Graphs

We consider the problem of classifying short sentences, where the sentences correspond to titles of products in e-commerce marketplaces such as Amazon, Etsy, and eBay. Automated product categorization is of interest because sellers may upload information corresponding to multiple listings, and may not be aware of the category tree the marketplace is using. It may be difficult for sellers to manually enter the appropriate category for each listing. A popular approach to solve such natural language processing (NLP) problems is to learn vector representations of words, subwords, or sentences and build classifiers. The subword model-based classifier in the fastText library is shown to be significantly faster than several deep neural network-based models and achieves comparable accuracy for a variety of NLP tasks, including single-sentence classification. In this work, we develop an alternate method that does not require learning vector representations of words. Our method works by constructing multiple weighted word co-occurrence graphs, one for each category. Given a new sentence/listing, we look for occurrences of the words in this sentence in each of the graphs, and predict the category based on a scoring heuristic. We show that for two publicly available datasets with millions of listings (from Etsy and Amazon), our approach achieves performance that is very close to a classifier built using the fastText library.

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11 - Reducing Memory Requirements of Quantum Optimal Control

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12 - Fast Tree-Based Algorithms for Dbscan on GPUs

DBSCAN is a well-known density-based clustering algorithm to discover clusters of arbitrary shape. The efforts to parallelize the algorithm on GPUs often suffer from high thread execution divergence (for example, due to asynchronous calls to range queries). In this poster, we propose a new general framework for DBSCAN on GPUs, and propose two tree-based algorithms within that framework. Both algorithms fuse neighbor search with updating clustering information, and differ in their treatment of dense regions of the data. We show that the cost of computing clusters is at most twice the cost of neighbor determination in parallel. We compare the proposed algorithms with existing GPU implementations, and demonstrate their competitiveness and excellent performance in the presence of a fast traversal structure (bounding volume hierarchy). In addition, we show that the memory usage can be reduced by processing the neighbors of an object on the fly without storing them.

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13 - Temporal Analysis of Epidemiology Indicators and Air Travel Data for Covid-19

Coronavirus Disease 2019 (Covid-19) is an ongoing outbreak and the latest threat to global health. It is imperative to understand the implications of social interaction on Covid-19 indicators in order to help formulate policies and guidelines by governments and local authorities. We present a case-study of curating state-level Covid-19 indicators such as Active Cases, Deaths, Hospitalization Rate, etc. for the United States. We also curate open source domestic USA air travel data and present its impact on Covid-19 indicators. We also perform a time-series analysis of the dataset using Independent Temporal Motif (ITeM) to find weekly trends in the data. We publish the dataset and the results for further exploration by the research community.

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14 - Scalable Approaches to Selecting Key Entities in Networked Infrastructure Systems

This work aims at bringing advances in discrete optimization algorithms to solving practical engineering problems at scale. Often times, in many engineering design problems, there is a need to select a small set of influential or representative elements from a large ground set of entities in an optimal fashion. Submodular optimization provides for a formal way to solve such problems. Common examples with infrastructure systems involve sensor placement and identification of key entities with certain objectives. However, scaling these approaches to large infrastructure systems can be challenging. In this work, we explore a well-studied and widely-applicable paradigm, namely leader-selection in a multi-agent networked setting in the context of scalable methodologies. We demonstrate novel frameworks that utilize variations of accelerated submodular optimization algorithms along with linear-algebraic methods that can help accelerate the oracle computations. We further explore this combination in conjunction with graph partitioning paradigms to take advantage of the accelerated algorithms in a distributed setting. Finally we demonstrate the key findings on a practical problem in a traffic control application, where we seek $k = 200$ key intersections. This problem can be solved in a serial setting in just under 5 hours providing more than 2 orders of magnitude speed-up over methods that do not consider acceleration techniques.

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15 - Towards Better Renyi Entropy Estimation

Estimation of Rényi entropy is of fundamental importance to many applications in cryptography, statistic or machine learning. This paper addresses some of the challenges with existing estimators, particularly the question about the sample size. The contribution is a novel analysis of the generalized "birthday paradox" collision estimator. The analysis is considerably simpler than in prior works, gives clear formulas and strengthens existing bounds. We use the improved bounds to study adaptive estimation, and show that it outperforms previous methods, particularly in regimes of low or moderate entropy. Last but not least, to demonstrate the usefulness of our techniques, a number of applications concerning theoretical and practical properties of "birthday estimators" is discussed.

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PP0

16 - Linear Time Algorithms for Edge Clique Cover of Graphs with Bounded Degeneracy

A set of cliques $\mathcal{C}$ is an edge clique cover of a graph if every edge of the graph is contained in at least one of the cliques in $\mathcal{C}$. Finding minimum cardinality edge clique cover is an NP-hard problem, and the problem does not admit constant-factor approximation algorithm unless $P = NP$. Edge clique cover is an abstraction of many real world problems, and for many of these problems, fast polynomial time algorithms are of paramount importance. We define a type of edge clique cover that admits desirable properties. Using theoretical foundations of the properties, we design a new framework of heuristic algorithms for computing edge clique cover. We describe fast instantiations of the framework. For a graph with degeneracy d and m edges, one such algorithm takes $O(md+|\mathcal{C}|d^2)$ time and $O(m+|\mathcal{C}|d)$ space. We further show that for many graph families, the algorithm can compute their solutions in $O(md)$ time, using $O(m)$ space. Our experiments show that our algorithms significantly outperform state-of-the-art heuristic algorithms for the problem, both on minimum cardinality objective and execution time. For real-world graphs (social networks, brain networks, gene regulatory networks) with billions of edges, the algorithms show linear dependence of computation time on number of edges. We also have applied the algorithms on a problem of improving neighbourhood communication patterns in MPI (message passing interface) library.

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PP0

17 - Conditional Preconditioning

In the field of combinatorial optimization preconditioning methods prove to be of crucial importance. We present a generic way of modifying some of these methods so that they are more effective in reducing the problem size. As an example we use the k-clique decision problem and two sets of kernelization methods. One set is based on coloring the neighborhood of a node or edge, the other is based on dominance of neighborhoods. We show that we can not only delete edges but put them back and thus delete more nodes and edges from the graph in the end. The presented method is versatile and can possibly be used in other examples as well.

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IP1

Opening Remarks and Presentation: Exploiting Redundancy in Nonlinear Optimal Control

Optimal Control provides the foundation for highly successful computational controller design methods such as model predictive control (MPC) or reinforcement learning (RL). However, even sophisticated computational approaches can only work if the complexity of the underlying optimal control problem is not too high. Methods that are able to tackle large-scale problems induced, e.g., by networked control systems or by discretized partial differential equations require some kind of redundancy of the underlying problem in order to be efficient. In this talk we will revisit two classical redundancy properties in nonlinear control and show why they are beneficial for modern computational methods. In the case of MPC, we will consider the turnpike property, a classical property of optimal control problems whose discovery goes back at least until the 1920s. We will show that the turnpike property explains why the receding horizon paradigm behind MPC works and that it allows for rigorous statements about stability, feasibility and near-optimal performance of MPC schemes. Concerning RL, we will argue that small-gain conditions, that are classical in linear control and were established in nonlinear control since the 1990s, can explain why deep neural networks can overcome the curse of dimensionality. We will investigate this property rigorously for a prototype problem of computing Lyapunov functions for nonlinear systems.

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IP2

Robustness in Machine Learning

Machine Learning (ML) hold a huge promise in many important applications, reshaping every aspect of our lives. Despite the promise and successful outcomes in applications that involve stationary environments, many existing ML algorithms fail drastically when data inputs or task objectives change from those used during algorithm training. Developing ML methods with robustness guarantees against such changes becomes even more crucial in the context of the safety critical applications. This talk will give an overview of ML methods and algorithms that can maintain performance in the presence of perturbations and gracefully adapt to changes in input data, task objectives and domain shifts. We will present new formulations and efficient training algorithms with both optimization and generalization guarantees that would be essential for safe and reliable deployment of ML technologies.

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IP3

Nevertheless it Persisted: Analyzing the Behavior of Epidemic Processes over Networks

The study of epidemic processes has been of interest over a wide range of fields for the past century, including in mathematical systems, biology, physics, computer science, social sciences and economics. There has been a resurgent interest in the study of epidemic processes focused on the spread of viruses over networks, motivated largely by recent outbreaks of infectious diseases, but also by the rapid spread of opinions over social networks, and the security threats posed by computer viruses. Many of the models considered in recent studies have been focused on network models with static network structures, however, frequently the systems being considered have inherently dynamic structures. In this talk we will discuss data-informed modeling, equilibria and convergence analysis results for epidemic processes over both static and time-varying networks, with the goal being to elucidate the behavior of such spread processes. Multi-strain/multi-virus models will also be discussed. Simulations and issues arising from the use of data from ongoing viral outbreaks will be reviewed to conclude the talk.

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IP4

Closing Remarks and Presentation: A Unified Approach to Convergence Analysis of Policy Update Methods for Control

Motivated by the widely used "policy gradients" and related methods that update a policy based on its observed cost (especially in reinforcement learning), the application of these methods to classical control design problems has been a recent focus of study. We start by examining these methods—their convergence and optimality—for the infinite-horizon Linear Quadratic Regulator (LQR), where we show that despite nonconvexity, gradient update methods converge to the optimal policy under mild assumptions. Next, we make a connection to classical convexification techniques, such as Youla parameterization—which leads to a unified way to prove similar results for a whole host of control design problems, as long as they admit a semidefinite programming representation.

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SP1

Best SICON Paper Prize Lecture #1: An Inexact Bundle Algorithm for Nonconvex Nonsmooth Minimization in Hilbert Space

We develop and analyze an inexact bundle method for nonsmooth nonconvex minimization on closed convex sets in infinite-dimensional Hilbert spaces. The proposed method requires only approximate (i.e., inexact) values of the cost function and of an element of the generalized differential. A quadratic term in the bundle subproblem allows to incorporate curvature information. We present a global convergence theory in a suitable infinite-dimensional Hilbert space setting. The method requires to control the inexactness in function evaluations and subproblem solves via accuracy conditions that are implementable. We illustrate our framework by applications to the optimal control of obstacle problems and present some numerical results.

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SP2

Best SICON Paper Prize Lecture #2: Controllability for Coupled Linear Parabolic PDEs

Coupled parabolic PDEs abound in the study of practical dynamical systems; for example, in atmospheric, epidemic, and biological system modeling. When tasked with regulating such systems, it is seldom the case that controls enter every equation within the system. This underactuation elicits the problem of determining whether such systems are controllable. Our work studies this controllability problem for systems governed by coupled linear parabolic PDEs that are controlled by interior inputs, where actuation is available on a limited number of subsystems, and where couplings appear as spatiallydistributed reaction and advectionlike terms. We provide an easily-verifiable sufficient controllability condition reminiscent of the Kalman rank condition for finite-dimensional systems, and in doing so, advance a control design technique that can be utilized to reduce the number of controls needed.

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SP3

SIAG/CST Prize Lecture: Capture the Structure: Parameter-free Analysis and Control of Dynamic Behaviours

Dynamical networks are composed of several subsystems that interact according to an interconnection topology. This broad class of systems includes not only multi-agent systems in engineering, but also natural systems in biology, ecology, epidemiology. Structural analysis aims at revealing properties of a dynamical network that are exclusively based on its structure (i.e., its topology along with qualitative assumptions) and are independent of parameter values, which are often uncertain or unknown. In particular, structural approaches can explain the extraordinary robustness that biological systems exhibit despite huge uncertainties and environmental fluctuations. We will introduce the BDC-decomposition as a local and global tool for structural analysis, which allows us to find criteria to structurally assess important properties, including the stability of equilibria and the sign of steady-state input-output influences. We will also discuss a structural classification of oscillatory and multistationary behaviours in systems that can be seen as the sign-definite interconnection of subsystems with suitable qualitative properties. We will finally illustrate how structural properties can be exploited for control purposes, and for the design of systems that are guaranteed to exhibit the desired behaviour even in highly uncertain environments.

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JP1

Joint Plenary Speaker with the 2021 SIAM Annual Meeting (AN21): Spiking Control Systems

Spikes are the heart beats of neuronal circuits, event-based cameras, and neuromorphic chips. How shall we control such systems? How shall we make them robust to uncertainty? How shall we design artificial spiking systems that will come even close to the efficiency, resilience, and learning capabilities of natural spiking systems? The control theory of spiking systems is in infancy. Neither analog, nor digital, nor hybrid theories properly acknowledge the distinct feature of spiking. This talk will discuss some of the core questions of spiking control and the potential of spiking communication for the future of control and computation.

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CP1

Error Bounds for Carleman Linearization of General Nonlinear Systems

In 1932, Carleman proposed his celebrated linearization method for transforming (lifting) a finite-dimensional nonlinear system with an analytic right-hand side into an equivalent infinite-dimensional linear system. One of the outstanding challenges with this method is that one usually has to deal with linear systems with unbounded operators, where a common approach to address this issue is to construct finite truncation of the infinite-dimensional system. It has been observed that the trajectory of the truncated system eventually diverges from the solution of the original nonlinear system, which raises several questions: what is the proper truncation size? How well does the truncated system approximate the original system? How long do the trajectories stay close to each other? This work provides explicit theoretical error bounds for the truncated system and proves that its trajectories stay close to the original nonlinear system over a quantifiable time interval. Moreover, if the original nonlinear system is asymptotically stable, the error vanishes as time goes to infinity. Our results hold for general time-varying nonlinear dynamical systems with analytic right-hand sides. To support our theoretical estimates, we will present several numerical case studies.

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CP1

Converse Lyapunov Theorems for Exponential Stability of Lipschitz Continuous Nonlinear Systems

It is proven that a necessary and sufficient condition for exponential stability of the zero equilibrium point of a Lipschitz continuous nonlinear system is existence of a Lyapunov function that is linearly bounded, and decreases monotonously along the system trajectories. This statement holds for both discrete and continuous time systems. Moreover, two different small gain theorems for discrete and continuous perturbed systems are given to demonstrate the potential of the given converse Lyapunov theorems. The addressed systems and Lyapunov functions are allowed to be nonsmooth. Hence, the present work can also be seen a contribution to nonsmooth analysis.

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CP1

Online Inner Approximation of Reachable Sets of Nonlinear Systems with Diminished Control Authority

This work presents a method of efficiently computing inner approximations of forward reachable sets for nonlinear control systems with diminished control authority, given an a priori computed reachable set for the nominal system. The method functions by shrinking a precomputed convex reachable set based on a priori knowledge of the system's trajectory deviation growth dynamics. The trajectory deviation growth dynamics determine an upper bound on the minimal deviation between two trajectories emanating from the same point that are generated by control inputs from the nominal and diminished set of control inputs, respectively. These growth dynamics are a function of a given Hausdorff distance bound between the nominal convex space of admissible controls and the possibly unknown impaired space of admissible controls. Because of its relative computational efficiency compared to direct computation of the off-nominal reachable set, this procedure can be applied to on-board fault-tolerant path planning and failure recovery. We consider the implementation of the approximation procedure by way of numerical integration and a root finding scheme, and we present two illustrative examples, namely an application to a control system with quadratic nonlinearities and aircraft wing rock dynamics.

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CP1

A Modified Fixed Point Methods for Controlling Dynamical Systems

In this work we treat in general non-linear dynamical systems. We give some results about the stable solutions of this type of equations and use a modified fixed point method to stabilize and control the system. In deed the resolution of the equations begins with an initial guess (that we don't know), we build a sequence that converge to the stable solution of our system if it exists. To have a good accuracy for the solution we treat, we apply an implicit scheme to this equation and use a modified fixed point technique to linearize our problem with a generalized nonlinear reaction and diffusion equation. Next, we apply this methods in particular to the the dynamical system of some chemical process. Several test-cases of analytical problems illustrate this approach and show the efficiency of the proposed new method.

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CP1

A Temporal Logic-Based Hierarchical Network Connectivity Controller

In this paper, we consider networks of static sensors with integrated sensing and communication capabilities. The goal of the sensors is to propagate their collected information to every other agent in the network and possibly a human operator. Such a task requires constant communication among all agents which may result in collisions and congestion in wireless communication. To mitigate this issue, we impose locally non-interfering communication constraints that must be respected by every agent. We show that these constraints along with the requirement of propagating information in the network can be captured by a Linear Temporal Logic (LTL) framework. Existing temporal logic control synthesis algorithms can be used to design correct-by-construction communication schedules that satisfy the considered LTL formula. Nevertheless, such approaches are centralized and scale poorly with the size of the network. We propose a hierarchical LTL-based algorithm that designs communication schedules that determine which agents should communicate while maximizing network usage. We show that the proposed algorithm is complete and demonstrate its efficiency and scalability through numerical experiments.

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CP1

Saddle Flow Dynamics: Observable Certificates and Separable Regularization

This paper proposes a certificate, rooted in observability, for asymptotic convergence of saddle flow dynamics of convex-concave functions to a saddle point. This observable certificate directly bridges the gap between the invariant set and the equilibrium set in a LaSalle argument, and generalizes conventional conditions such as strict convexity-concavity and proximal regularization. We further build upon this certificate to propose a separable regularization method for saddle flow dynamics that makes minimal requirements on convexity-concavity and yet still guarantees asymptotic convergence to a saddle point. Our results generalize to saddle flow dynamics with projections on the vector field and have an immediate application as a distributed solution to linear programs.

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CP2

Observer Design and Temperature Regulation of a Catalytic Reverse Flow Reactor Distributed Parameter Model

In this work, control and estimation problems have been

studied for a catalytic reversal flow reactor (CFRR). A stabilizing compensator is developed on the basis of the infinite-dimensional state-space description of the CFRR. Linear-quadratic technique is used to design both an optimal state-feedback controller and an output injection operator. The developed compensator is tested numerically for the catalytic combustion of lean methane emissions.

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CP2

Approximate Controllability of Nonlocal and Impulsive Integro-Differential Equations of Finite Delay

In this lecture, we derive sufficient conditions for the approximate controllability of nonlocal and impulsive integro-differential equations of finite delay using the resolvent operator theory in a Hilbert space. For this, we first convert the controllability problem into a fixed point problem to show the existence of a mild solution of the system and then establish the approximate controllability of the system. The main tools applied in our analysis are semigroup theory, the resolvent operator theory, fractional power theory, Krasnoselskii's fixed point theorem, and Schauder's fixed point theorem. Finally, we provide an example to show the application of our main results.

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CP2

Viscosity Solutions of Hamilton-Jacobi-Bellman PDEs for Fractional-Order Systems

We consider optimal control problems for systems governed by fractional differential equations of Caputo type. In addition to memory properties due to fractional derivatives, we suppose that the vector fields and costs depend on past histories of state trajectories. We define value functions as functionals of past state trajectories and show that they satisfy path-dependent dynamic programming principles. Using co-invariant derivatives of fractional type, we propose a viscosity solution notion for nonlinear PDEs with co-invariant derivatives of fractional type. We show that the value functionals are unique viscosity solutions for Hamilton-Jacobi-Bellman PDEs derived from the path-dependent dynamic programming principles.

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CP2

Approximate Controllability from the Exterior of Space-Time Fractional Parabolic-Elliptic Coupled Systems

We study the approximate controllability of the following parabolic-elliptic coupled system involving the fractional Laplacian $(-\Delta)^s$, $s \in (0,1)$,

$$\begin{cases} \partial_t u + (-\Delta)^s u = au + bv \text{ in } \Omega \times (0,T), \\ (-\Delta)^s v = cu + dv \text{ in } \Omega \times (0,T), \\ u = g1_{\mathcal{O}},\ v = 0 \text{ in } (\mathbb{R}^N \setminus \Omega) \times (0,T), \\ u(.,0) = u^0 \text{ in } \Omega, \end{cases} \tag{1}$$

and of a similar system to (1) with the following exterior Dirichlet condition $u = 0$, $v = h1_{\mathcal{O}}$ in $(\mathbb{R}^N \setminus \Omega) \times (0,T)$ with $a, b, c, d \in \mathbb{R}$. The controls g and h are located on a nonempty open subset $\mathcal{O}$ of the complementary of the open bounded domain Ω in $\mathbb{R}^N$. For this reason, the approximate controllability is said to be exterior. To obtain the controllability properties, we first prove the existence and uniqueness of the series solution of the studied systems and their dual. Then we state a unique continuation principle for the dual equation which follows from a unique continuation property for the eigenvalues of $(-\Delta)^s$ with the homogeneous exterior Dirichlet condition. Finally, we show that for any $s \in (0,1)$ and any control in $C_c^\infty(\mathcal{O} \times (0,T))$, under certain conditions on the coefficients, the approximate controllability at any time $T > 0$ holds.

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CP2

Mixed Monotone Iterative Technique for Impulsive Hilfer Fractional Evolution Equations

The well established mixed monotone iterative technique that is used to study the existence and uniqueness of fractional impulsive system is extended to Hilfer fractional order in this paper. The results are derived by using the method of upper and lower quasi-solution and C_0-semigroup. Also, conditions on non-compactness of measure is used effectively to prove the main result. An illustrative example is also presented. Recent results from the work of "Haide Gou, Monotone iterative technique for Hilfer fractional evolution equation with non-local conditions" and "Jing Zhao & Rui Wang, Monotone iterative technique for fractional impulsive evolution equations" are used as main references.

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CP2

Approximate Controllability of Riemann-Liouville Fractional Order Systems with Non-Instantaneous Impulses

The study is dedicated towards Riemann-Liouville fractional order differential equations with non-instantaneous impulses. Firstly, the uniqueness and existence of solutions are proven using fixed point approach. Then approximate controllability for the system is examined. The motivation of the work is mainly due to two reasons, one is the property of non-instantaneous impulses which starts all at once but holds for a finite time interval. The other is lesser availability of literature on study of non-instantaneous impulses associated with Riemann-Liouville derivatives. The considered system is:

$$D_t^\eta z(t) = Az(t) + Bu(t) + g(t, z(t)), \qquad t \in \cup_{i=0}^{n}(p_i, t_{i+1}],$$
$$z(t) = \Im_i(t, z(t_i^-)), \quad t \in (t_i, p_i], \quad i = 1, 2, ..., n,$$
$$I_t^{1-\eta} z(t)|_{t=0} = z_0 \in Z,$$

where D_t^η denotes the Riemann-Liouville derivative of order η, $0 < \eta < 1$, the constants p_i and t_i satisfy the relation $0 = p_0 = t_0 < t_1 < p_1 < t_2 < ... < p_n < t_{n+1} = T$, and $\Im_i$ and g are functions to be specified later. $A : D(A) \subseteq Z \to Z$ is the infinitesimal generator of a C_0-semigroup $T(t)(t > 0)$ on the Banach space Z. B is a linear operator and $z(t)$ and $u(t)$ belong to Banach spaces Z and U respectively.

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CP3

Quantitative Resilience of Linear Driftless Systems

This paper introduces the notion of quantitative resilience of a control system. Following prior work, we study linear driftless systems enduring a loss of control authority over some of their actuators. Such a malfunction results in actuators producing possibly undesirable inputs over which the controller has real-time readings but no control. By definition, a system is resilient if it can still reach a target after a partial loss of control authority. However, after such a malfunction, a resilient system might be significantly slower to reach a target compared to its initial capabilities. We quantify this loss of performance through the new concept of quantitative resilience. We define such a metric as the maximal ratio of the minimal times required to reach any target for the initial and malfunctioning systems. Nave computation of quantitative resilience directly from the definition is a complex task as it requires solving four nested, possibly nonlinear, optimization problems. The main technical contribution of this work is to provide an efficient method to compute quantitative resilience. Relying on bang-bang control theory and on two novel geometric results we reduce the computation of quantitative resilience to a single linear optimization problem. We demonstrate our method on an opinion dynamics scenario.

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CP3

Time-Optimal Coordination for Connected and Automated Vehicles at Adjacent Intersections

Traffic congestion has become a significant concern in big metropolitan areas. By 2050, it is expected that 68% of the population will reside in urban areas. In 2017, congestion in urban areas in the US caused drivers to spend an extra 8.8 billion hours on the road and purchase an extra 3.3 billion gallons of fuel resulting in $166 billion cost. In addition, about 35K people in the US lose their lives in traffic accidents each year. One of the promising ways to mitigate congestion and improve safety is the integration of information and communication technologies with cities. Using connected and automated vehicles (CAVs) is one of the intriguing ways towards transitioning to smart cities. In this talk, we present a decentralized optimal control framework for CAVs crossing two adjacent intersections. The framework consists of an upper-level scheduling problem and a low-level optimal control problem. The solution of the upper-level problem designates the optimal time of each CAV aimed at minimizing its travel time to cross the intersections. The outcome of the upper-level scheduling problem becomes the input of the low-level problem, the solution of which yields the optimal control input (acceleration/deceleration) of each CAV to exit the intersections at the time specified in the upper-level scheduling problem. We demonstrate the effectiveness of the proposed framework through numerical simulation.

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CP3

Mean Field Models to Regulate Carbon Emission Levels in Electricity Production

The most serious threat to ecosystems is the global climate change fueled by the uncontrollable increase in the carbon emission levels. In this project, mean-field control and mean-field game models are proposed to analyze the decision of electricity producers on how much nonrenewable and renewable energy resources to use in the electricity generation and the influence of carbon tax policies imposed by a regulator on this decision. The trade-off between higher levels of revenue from electricity production and the negative effects of carbon emission on the environment affects electricity producers decisions to choose how much cheaper, reliable but polluting nonrenewable energy or clean but random renewable energy to use in production. We compare these decisions under two different settings where the producers are competitive (Nash Equilibrium) or cooperative (Social Optimum) and we further analyze the Stackelberg Equilibrium with the addition of a regulator that decides on the carbon tax levels.

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CP3

Learning Shape Control of Multi-Agent Systems with Lagrangian Neural Networks

Shape control of double integrator agents can be seen as a stabilization system whose evolution can be described by forced Euler-Lagrange equations. If agents are subject to unknown disturbances, desired shapes can not be achieved with the classical controllers. We propose a Neural Network for forced Lagrangian systems to learn the unknown disturbances, and we use the learning to re-design the controller to achieve the desired shape. A numerical example highlights the effectiveness of the proposed learning-based control law.

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CP3

Resource Allocation for Prioritization and Gating of Memory Traces in Linear Systems

When presented with stimuli, internal processes within the brain must somehow determine which, if any, of this information to retain, and which to ignore in order to prevent redundancy or exceed its available resources. The process and mechanisms the brain uses to vet the stimuli it receives is still greatly unknown and a long-standing research question in brain science. Here, we use a linear dynamical systems framework, treating the state trajectory as a memory trace of prior inputs, to study hypothetical mechanisms for how neural circuits might allocate resources to incoming stimuli. We propose and formulate the concept of importance of stimuli as a quantitative representation of relevance to anticipated events. Using this notion of importance as well as the size of incoming signals, we define a cost function to be used by the system to balance the need to gather important stimuli with the demands of practicality. Minimizing this cost, we derive a decision policy that allows the network to determine whether and how a given input should impinge on the system, allocating its finite resources optimally. We show that this decision policy is biophysically interpretable, insofar as subnetworks can independently accept or reject each stimulus and still achieve the global optimal solution.

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CP3

A Nonzero-Sum Game Formulation for a Markov Regime-Switching Portfolio Strategy

We apply dynamic programming principle to discuss an optimal investment problems by nonzero-sum stochastic game approach in a continuous-time Markov regime-switching environment. We represent different states of an economy or investors floating levels of psychologica by a D-state Markov chain. We formulate a nonzero-sum stochastic differential portfolio game as the sensitivity of two investors terminal gains.We derive regime-switching HamiltonJacobiBellmanIsaacs equations and obtain explicit optimal portfolio strategies with FeynmanKac representations of value functions.We illustrate our results in a two-state special case and observe the impact of regime switches by comparative results.

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CP4

On the Rare-Event Simulations of Diffusion Processes Pertaining to a Chain of Dynamical Systems with Small Random Perturbations

In this talk, we consider an importance sampling problem for a certain rare-event simulations involving the behavior of a diffusion process pertaining to a chain of dynamical systems with small random perturbations. Here we assume that the dynamical system formed by n-subsystems - in which a small random perturbation enters in the first subsystem and then subsequently transmitted to the other subsystems - satisfies an appropriate Hörmander condition. We provide an efficient importance sampling estimator for the asymptotics of the probabilities of the rare events involving such a diffusion process that ensures a minimum relative estimation error in the small noise limit. The framework for such an analysis relies on the connection between the probability theory of large deviations and the values functions for a family of stochastic control problems associated with the underlying system, where such a connection provides a computational paradigm - based on an exponentially-tilted biasing distribution - for constructing efficient importance sampling estimators for the rare-event simulation. As a by-product, the framework allows us to derive a family of Hamilton-Jacobi-Bellman for which we also provide a solvability condition for the corresponding optimal control problem. Moreover, the applicability of the proposed framework is demonstrated through diffusion processes pertaining to an opioid epidemic dynamical model with small random perturbations.

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CP4

Nonlinear Two-Time-Scale Stochastic Approximation: Convergence and Finite-Time Performance

Two-time-scale stochastic approximation, a generalized version of the popular stochastic approximation, has found broad applications in many areas including stochastic control, optimization, and machine learning. Despite of its popularity, theoretical guarantees of this method, especially its finite-time performance, are mostly achieved for the linear case while the results for the nonlinear counterpart are very sparse. Motivated by the classic control theory for singularly perturbed systems, we study in this paper the asymptotic convergence and finite-time analysis of the nonlinear two-time-scale stochastic approximation. Under some fairly standard assumptions, we provide a formula that characterizes the rate of convergence of the main iterates to the desired solutions. In particular, we show that the method achieves a convergence in expectation at a rate $O(1/k^{2/3})$, where k is the number of iterations. The key idea in our analysis is to properly choose the two step sizes to characterize the coupling between the fast and slow-time-scale iterates.

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CP4

Inverse Stochastic Optimal Controls

We study an inverse problem of the stochastic control of general diffusions with performance index having the quadratic penalty term of the control process. Under mild conditions on the drift, the volatility, the cost functions of the state, and under the assumption that the optimal control belongs to the interior of the control set, we show that our inverse problem is well-posed. Then, with the well-posedness, we reduce the inverse problem to some root finding problem of the expectation of a random variable involved with the value function, which has a unique solution. Based on this result, we propose a numerical method for our inverse problem by replacing the expectation above with arithmetic mean of observed optimal control processes and the corresponding state processes. Several numerical experiments show that the numerical method recover the unknown weight parameter with high accuracy.

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CP4

Execution Shortfall Algorithms under Regime Switching

This paper is concerned with the problem of trading a large position in the market place when the stock price follows a regime-switching process. In this work, we are particularly interested in trading algorithms that minimize the execution shortfall. The underlying problem is formulated as a discrete-time stochastic optimal control problem with resource constraints. The value function and optimal trading strategies are derived in closed-form. Numerical simulations with market data are reported to illustrate the pertinence of these results.

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CP4

Optimal Multi-Target Path Planning in Markov Decision Processes

Visiting multiple targets is a common path planning scenario in various autonomous missions. In this work, we model the environment as a Markov decision process, and aim to find a control policy that minimizes the expected time to reach a set of target states. By reducing our problem to a Hamiltonian path problem, we show that ours is at least NP-complete. Using Bellman's optimality equation, we present an optimal algorithm that is exponential in the number of target states. Then, we trade-off optimality for time complexity by presenting an algorithm that is polynomial at each time step. We prove that the proposed suboptimal procedure generates optimal policies for certain types of Markov decision processes. We compare the performance of our algorithms with previous approaches, and show that ours produce better results on random Markov decision processes, as well as on a gridworld environment inspired by autonomous underwater vehicles operating in an ocean.

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CP5

A New Perspective for Offline LQ Optimal Control: the LQ Reproducing Kernel and Its Relation to the Dual Riccati Equation

We provide an interpretation of the dual differential Riccati equation of Linear-Quadratic (LQ) optimal control problems. Adopting a novel viewpoint, we show that LQ optimal control can be seen as a regression problem over the space of controlled trajectories, and that the latter has a very natural structure as a reproducing kernel Hilbert space (RKHS). When initial and final times are fixed, the corresponding LQ kernel shines a new light on classical control notions, such as the Gramian of controllability. When the initial time changes, the dual Riccati equation describes the evolution of the values of the LQ reproducing kernel. Whereas the solution $J(\cdot, T)$ of the differential Riccati equation maps the optimal trajectory $\bar{x}(\cdot)$ to its adjoint vector $p(\cdot)$, the kernel $K(\cdot, t_0)$ maps an initial covector p_0 to the optimal trajectory $\bar{x}(\cdot)$. This effectively inverts the graph of the relation between $\bar{x}(\cdot)$ and $p(\cdot)$. The inversion performed is related to a general change of perspective, from an online and differential approach to an offline and integral one, more suitable for optimal synthesis. This unveils new connections between control theory and kernel methods, a field widely used in machine learning.

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CP5

Toward Analytical Solutions of Constraint-Driven Optimal Planning Problems

In this work, we present our recent results in optimal planning for constraint-driven agents. There has been a growing interest in constraint-driven systems recently, i.e., energy-minimizing agents with a feasible action space that describes the admissible control actions. This approach is advantageous for long-duration autonomy tasks, where an agents behavior is closely tied to the uncertain dynamics of the environment. To this end, we have derived several key results for energy-optimal planning by constraint-driven agents. First, we demonstrate that differential flatness, i.e., invertibility of the agent dynamics, is sufficient to decouple the forward-backward equations that emerge from Hamiltonian analysis. This result enables the agent to generate the energy-optimal trajectory independent of the costate dynamics, reducing the agents computational load. Next, we show that continuity in the control input is an equivalent optimality condition for integrator systems in some instances. This result allows us to decouple the boundary and interior conditions from the costate dynamics; thus, numerical shooting methods become a feasible technique to generate energy-optimal trajectories with constraint activations. We also present a class of self-relaxing constraints that improve the robustness of the constraint-driven optimal control approach. Finally, we demonstrate our results in simulation using a multi-agent environment.

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CP5

Deep Reinforcement Learning Initialization and Acceleration of Direct Collocation Optimal Control Problems Solvers

Direct collocation has become one of the main approaches we use to solve optimal control problems in practice. High accuracy requirements create the demand to make such solvers as performant as possible. However, the accuracy and convergence rate of direct collocation solvers is known to depend on the quality of their initialization. Recently we saw the successful application of deep reinforcement learning algorithms to several optimal control tasks. Such algorithms provide an efficient method for fast initialization near globally optimal solutions. We thus propose the use of deep Q networks to generate initial solutions for collocation algorithms.

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CP5

Optimal Time Trajectory and Coordination for Connected and Automated Vehicles

Connected and automated vehicles (CAVs) provide the most intriguing opportunity for enabling users to better monitor transportation network conditions and make better operating decisions to improve safety and reduce pollution, energy consumption, and travel delays. As we move to increasingly complex emerging mobility systems, new control approaches are needed to optimize the impact on system behavior of the interplay between vehicles at different traffic scenarios. In this talk, I will present a decentralized control framework for coordination of CAVs in different traffic scenarios, e.g., merging at roadways and roundabouts, crossing unsignalized intersections. The framework includes: (1) an upper-level optimization that yields for each CAV its optimal path, including the time and lane, to pass through a given traffic scenario by alleviating congestion; and (2) a low-level optimization that yields for each CAV its optimal control input (acceleration/deceleration) to achieve the optimal path and time derived in the upper-level. I will present a geometric duality framework using hyperplanes to prove strong duality of the upper-level optimization problem and the condition under which the optimal solution always exists. Strong duality implies that the optimal path for each CAV does not activate any of the state, control, and safety constraints of the low-level optimization, thus allowing for online implementation.

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CP5

Results on Optimal Control for Abstract Semilinear Second-Order Systems

The article provides sufficient conditions for optimal control of the second-order semilinear system in abstract space. In this article, we convert the second-order system into a first-order simultaneous system of equations and derive sufficient conditions for the optimal control of the first-order system. As both the systems are equivalent, the second-order system also follows the optimal control. Also, time-optimal control is discussed.

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CP5

Well-Posedness of History/State-Dependent Implicit Sweeping Processes

This talk is devoted to present a new class of implicit state-dependent sweeping processes with history-dependent operators. Based on the methods of convex analysis, we prove the equivalence of the history/state dependent implicit sweeping process and a nonlinear differential equation, which, through a fixed point argument for history-dependent operators, enables us to prove the existence, uniqueness, and continuous dependence of the solution in a very general framework. Moreover, we present some new convergence results with respect to perturbations in the data, including perturbations of the associated moving sets. Finally, the theoretical results are applied to prove the well-posedness of a history-dependent quasi-static contact problem.

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MS1

Error Bounds for Port-Hamiltonian Reduced-Order Controllers

Linear quadratic Gaussian (LQG) control design for port-Hamiltonian systems is studied. A recently proposed method from the literature is reviewed and modified such that the resulting controllers have a port-Hamiltonian (pH) realization. Based on this new modification, a reduced-order controller is obtained by truncation of a balanced system. The approach is shown to be closely related to classical LQG balanced truncation and shares a similar a priori error bound with respect to the gap metric. With regard to this error bound, a theoretically optimal pH-representation is derived. Consequences for pH-preserving balanced truncation model reduction are discussed and shown to yield two different classical $\mathcal{H}_\infty$-error bounds.

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MS1

Optimal Feedback Law Recovery by Gradient-Augmented Sparse Polynomial Regression

A sparse regression approach for the computation of high-dimensional optimal feedback laws arising in deterministic nonlinear control is proposed. The approach exploits the control-theoretical link between Hamilton-Jacobi-Bellman PDEs characterizing the value function of the optimal control problems, and first-order optimality conditions via Pontryagin's Maximum Principle. The latter is used as a representation formula to recover the value function and its gradient at arbitrary points in the space-time domain through the solution of a two-point boundary value problem. After generating a dataset consisting of different state-value pairs, a hyperbolic cross polynomial model for the value function is fitted using a LASSO regression. An extended set of low and high-dimensional numerical tests in nonlinear optimal control reveal that enriching the dataset with gradient information reduces the number of training samples, and that the sparse polynomial regression consistently yields a feedback law of lower complexity.

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MS1

Balanced Truncation Model Reduction via Nonlinear Energy Functions

Balanced truncation model reduction uses the input and output energies of a systems to determine which states are relatively more important than others. The theoretical foundation proposed by Scherpen in the 1990s defines input and output energy functions and shows that they can be computed by solving Hamilton-Jacobi partial differential equations. The computation of balancing transformations for nonlinear large-scale systems remains an immense challenge. In this talk, we discuss polynomial approximation-based computation of the energy functions and nonlinear state transformations, which are scalable via tensor methods to large-scale systems. We then derive reduced-order models. We present numerical results on Burgers equation and other nonlinear test problems.

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MS1

Model Reduction of Monotone Nonlinear Systems by Dc Gains

In this presentation, we develop data-driven model reduction methods for monotone nonlinear control systems based on a nonlinear version of the dc gain. The nonlinear dc gain is a function of the amplitude of the input and can be used to evaluate the importance of each state variable. In fact, the nonlinear dc gain is directly related to the infinity-induced norm of the system as well as a notion of output reachability. Given the dc gain, model reduction is performed by either truncating not-so-important state variables or aggregating state variables having similar importance. Under such truncation and clustering, monotonicity and boundedness of the nonlinear dc gain are preserved; moreover, these two operations can be approximately performed based on simulation or experimental data alone. This empirical model reduction approach is illustrated by an example of a gene regulatory network.

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MS2

Regularized and Distributionally Robust Data-Enabled Predictive Control

We study the problem of finite-time constrained optimal control of unknown systems. We propose a novel distributionally robust data-enabled predictive control (DeePC) algorithm which uses noise-corrupted input/output data to predict future trajectories and compute optimal control inputs while satisfying output chance constraints. The algorithm is based on (i) a non-parametric representation of the subspace spanning the system behaviour, where past trajectories are sorted in Page or Hankel matrices; and (ii) a distributionally robust optimization formulation which gives rise to strong probabilistic performance guarantees. We show that for certain objective functions, DeePC exhibits strong out-of-sample performance, and at the same time respects constraints with high probability. We illustrate our results with nonlinear noisy simulations and experiments in an aerial robotics case study.

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MS2

Wasserstein Distributionally Robust Risk Map for Learning-Based Motion Planning and Control: A Semidefinite Programming Approach

Motion planning and control are considered to be fundamental problems in today's robotics as robots are making their way into the cluttered urban environment where humans inhabit. Therefore, a crucial task is constructing a path for the robot and controlling it to track the given reference, considering the dynamic and possibly uncertain behavior of the environment. State-of-the-art learning techniques enable predicting the uncertainties in the perceived information about surroundings, making the operation of the robots more intelligent. The difficulty arises when the environment changes rapidly and predictions about its future realizations might be inaccurate. To tackle this issue, we present a novel risk map for learning-based mobile robots, that is robust against distributional uncertainties of the environment. The proposed tool first learns the obstacles' unknown motion from observations using Gaussian Process Regression, then limits the risk of unsafety of the system given the learning results. This is accomplished by considering the worst-case risk of collision within an ambiguity set constructed as a statistical ball centered at the learned distribution. The resulting risk map, formulated as a semidefinite program, can be used in various motion planning and control algorithms, such as RRT* and MPC to ensure the safe navigation of the robot.

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MS2

Improved Decision Rule Approximations for Multi-Stage Robust Optimization via Copositive Programming

We study decision rule approximations for generic multi-stage robust linear optimization problems. We consider linear decision rules for the case when the objective coefficients, the recourse matrices, and the right-hand sides are uncertain, and consider quadratic decision rules for the case when only the right-hand sides are uncertain. The resulting optimization problems are NP-hard but amenable to copositive programming reformulations that give rise to tight conservative approximations. We further enhance these approximations through new piecewise decision rule schemes. Finally, we prove that our proposed approximations are tighter than the state-of-the-art schemes and demonstrate their superiority through numerical experiments.

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MS2

Towards Integrated Perception and Motion Planning with Distributionally Robust Risk Constraints

Safely deploying robots in uncertain and dynamic environments requires a systematic accounting of various risks, both within and across layers in an autonomy stack from perception to motion planning and control. Many widely used motion planning algorithms do not adequately incorporate inherent perception and prediction uncertainties, often ignoring them altogether or making questionable assumptions of Gaussianity. This talk describes a distributionally robust incremental sampling-based motion planning framework that explicitly and coherently incorporates perception and prediction uncertainties. The framework produces output feedback policies based on moment-based ambiguity sets of distributions to enforce probabilistic collision avoidance constraints under the worst-case distribution in the ambiguity set. Our solution approach, called Output Feedback Distributionally Robust RRT*(OFDR-RRT*), produces asymptotically optimal risk-bounded trajectories and policies for robots operating in dynamic, cluttered, and uncertain environments, explicitly incorporating mapping and localization error, stochastic process disturbances, unpredictable obstacle motion, and uncertain obstacle locations. The talk will discuss emerging issues including nonlinear control and filtering algorithms, dynamic ambiguity sets, and incorporation of learning algorithms.

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MS3

Uniqueness and Structure of Kinematic Chains

Kinematic chains play a central role in the design and calibration of industrial robotics. In essence, industrial robots attach their "end effector" to an object, reposition and reorient the object, and then release it; repeating any number of such operations as determined by a program. That is, they generate sequences of displacements in $\mathbb{R}^3$. In many cases the physical motion is implemented by a "chain", consisting of rigid links connected, one to the next, using a motorized single degree of freedom joint. If there are six such joints, and if the attachment angles are sufficiently different, then such a device can generate a rich subset of the set of all elements of $SE(3)$, the six-dimensional Euclidean group. As is standard, we associate with a rigid displacement of the form $x \mapsto \Theta x + d$ a matrix

$$T = \begin{bmatrix} \Theta & d \\ 0 & 1 \end{bmatrix}$$

This leads to the description of the motion generated

$$\begin{bmatrix} \Theta & d \\ 0 & 1 \end{bmatrix} = e^{A_1 x_1} e^{A_2 x_2} \cdots e^{A_6 x_6}$$

with x_i representing the programmable joint angles and the A_i, elements of the Lie algebra of $SE(3)$, determined by the geometry of the chain.

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MS3

Practical Reinforcement Learning for Robotics in the Presence of Symmetries

When a mechanical system exhibits a symmetry, the system's dynamics can often be realized in a reduced form that simplifies the interpretation of these dynamics or facilitates the synthesis of relevant control policies. The mathematical formalism for reduction in the presence of symmetries was developed in the context of systems with fully modeled dynamics, but a system's dynamics can be known to exhibit a symmetry associated, for instance, with an obvious conservation law even if an explicit dynamic model is unavailable. A control policy for a system with unmodeled dynamics can often be developed algorithmically though some form of reinforcement learning, but the practical success of such an approach depends on its computational complexity, which depends in turn on issues of dimensionality, motivating dimensional reduction whenever possible. When reinforcement learning is applied in the context of a robotic system, the system's dynamics and the control objective may exhibit distinct independent symmetries, both of which affect reducibility. This talk will outline basic features of this problem, illustrated with examples involving both continuous and discrete symmetries.

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MS3

Why Is Geometric Control Theory So Difficult?

Problems in geometric control theory having to do with the structure of the reachable set are notoriously challenging. While a great deal of progress has been made, and important and general theorems have been proved to answer certain questions, e.g., the Orbit Theorem, the fact remains that a comprehensive understanding of some of the most fundamental questions remains absent. In this talk we will discuss some reasons why such problems as controllability, stabilisability, and optimality remain unresolved. The emphasis is on difficulties associated with flows.

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MS3

Liouville Geometry and Control of Thermodynamic Systems

Since the early 1970s contact geometry has been recognized as a natural framework for the geometric formulation of classical thermodynamic systems. As initiated one can go further by replacing the intensive variables by their homogeneous coordinates, and thus formulating thermodynamics on the cotangent bundle of the space of external variables. This construction, known in differential geometry, has several advantages, including the unification of the energy and entropy representation of thermodynamic systems. Furthermore, it leads to the definition of port-thermodynamic systems. The underlying geometry can be called Liouville geometry, since all notions (submanifolds, vector fields, ports) are defined in terms of the Liouville form on the cotangent bundle. We consider the control of thermodynamic systems by shaping by feedback the system into a desired thermodynamic system.

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MS4

Fast and Safe Charging of Li-Ion Batteries via Closed-Loop Control

This talk presents a closed-loop control strategy based on Reference Governors (RG) for safe and fast charging of lithium-ion batteries and its experimental validation. Although battery rapid charging has been the subject of much research in recent years, mitigating battery aging while charging has been barely accounted for. The latter issue is overriding if degradation mechanisms like lithium plating occur, which can compromise the safe use of the battery. The proposed control scheme consists of two parts, both of them exploiting a reduced electrochemical model. The first part uses a linear quadratic regulator to push the battery (fast) charging performance. The second part resorts to a RG to handle electrochemical constraints that enforce the proper (safe) operation of the battery. Since these constraints define a nonconvex region, a novel computationally efficient formulation of the RG was derived. The proposed feedback charge strategy was experimentally validated and contrasted with commercially available and widely used charging strategies such as constant-current/constant-voltage (CCCV). The proposed approach charges the battery faster than a high current CCCV while degrading its capacity as much as a mild current CCCV over one hundred full charge/discharge cycles. These encouraging results highlight the conservativeness and even dangerousness of standard charging strategies obtained from empirical evidence with respect to physics-based control theoretic approaches.

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MS4

Real-Time Detection and Estimation of Thermal Faults in Batteries

This talk will present online algorithm for detection and estimation of thermal faults in batteries. Batteries are promising candidates for energy storage solutions in renewable power grids, electrified transportation and consumer electronics. However, the current battery technologies still suffer from safety issues. Online battery management algorithms have the potential to significantly improve battery safety. In this context, we will discuss how to design real-time algorithms for battery diagnostics by combining system-theoretic tools and physics-based battery models. Specifically, the algorithm is based on Partial Differential Equation (PDE) filtering techniques and distributed parameter thermal model that captures temperature distribution in battery cells. We will illustrate the effectiveness of the algorithms via experimental and simulation studies.

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MS4

Analysis and Optimization of Input and Output Data for Estimation of Battery States and Parameters

Estimation of battery internal states and parameters is one of the most important tasks of battery management. Estimation typically involves 3 basic elements, i.e. model, algorithm and data (e.g. current, voltage, and temperature measurements). While substantial efforts have been devoted to model development and algorithm design, our interest focuses on exploring the role of data in estimation, e.g. what are the optimal data pattern that would yield the best estimation accuracy? We will first demonstrate data optimization using the Fisher information criterion, which is the traditional gold standard for optimal experiment design, based on our analytically derived sensitivity expression of battery parameters. We will then show that such approach suffers major limitations including inability to address system uncertainties. We will then present our recently discovered data structures that relate estimation errors to system uncertainties. By incorporating these data structures for data optimization, the accuracy of estimation can be dramatically improved under system uncertainties (by up to 1 order of magnitude). Based on these data structures, we are developing a new set of criteria and framework applicable to a variety of data-optimization-for-estimation problems, including optimal experiment design and parameter management for system identification, and data selection/mining (from passive data stream) for online estimation.

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MS4

PDE Observer for All-Solid-State Batteries via an Electrochemical Model

All-solid-state batteries (ASSB) are one of the most promising candidates for next-generation energy storage devices capable of delivering higher specific energy. Significant efforts have been spent on understanding and controlling the degradation mechanisms associated with dendrite formation, while energy management and model-based control/estimation for solid-state batteries has received very limited attention. This talk presents a partial differential equation (PDE) state estimation scheme for a one-dimensional electrochemical all-solid-state battery model, using only voltage and current measurements. Knowledge on real-time electrochemical information will enable high-fidelity internal state estimation and optimal control in advanced battery management systems. By assuming a uniform lithium-ion concentration in solid electrolyte and compensating the neglected component with a boundary disturbance in the electrode dynamics, we propose an asymptotically convergent state estimation algorithm using concepts from active disturbance rejection control and PDE backstepping technique. The key novelty lies in proposing the first PDE estimator for electrochemical model-based monitoring that identifies physical variables for all-solid-state batteries.

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MS5

High-Dimensional Hamilton-Jacobi PDEs with State-Dependent Hamiltonians Arising from Certain Optimal Control Problems

We present analytical solutions for certain optimal control problems, where the running cost depends on the state variable. An analogue of the Lax-Oleinik representation formula is provided for the corresponding Hamilton-Jacobi PDEs, where the Hamiltonian also depends on the state variable. We propose efficient optimization-based algorithms for solving these optimal control problems and Hamilton-Jacobi PDEs in high dimensions. Numerical experiments show that our algorithms are suitable for numerically solving these optimal control problems in high-dimensional real-time applications.

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MS5

Improving Reliability in Neural Network Optimal Feedback Control Design

Recent work has demonstrated the potential of supervised learning as an effective method for solving high-dimensional Hamilton-Jacobi-Bellman equations, which arise in optimal feedback control. In this talk we discuss further developments to these methods to improve robustness during learning and enhance stability properties of the learned controller. Concretely, we augment neural network controllers with linear quadratic regulators to improve local stability and scaffold learning. We apply the proposed method to design candidate optimal feedback controllers for high-dimensional and unstable nonlinear systems, and through these examples, demonstrate improved reliability and accuracy compared to existing neural network formulations.

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MS5

Interior Point Differential Dynamic Programming

This work introduces a novel Differential Dynamic Programming (DDP) algorithm for solving discrete-time finite-horizon optimal control problems with inequality constraints. Two variants, namely Feasible and Infeasible Interior Point Differential Dynamic Programming (IPDDP) algorithms, are developed using primal-dual interior-point methodology, and their local quadratic convergence properties are characterised. We show that the stationary points of the algorithms are the perturbed KKT points, and thus can be moved arbitrarily close to a locally optimal solution. While general purpose primal-dual interior-point methods are successful in practice, there were no extension of the DDP algorithm accommodating primal-dual interior-point techniques reported so far. Our aim is to fill this gap. The proposed IPDDP framework is a natural extension to DDP. It requires neither modifying the objective function nor identifying active/inactive constraints by a separate procedure. Being free from the burden of active-set methods, it can handle nonlinear state and input inequality constraints without a discernible increase in its computational complexity relative to the unconstrained case. The performance of the proposed algorithms is demonstrated using numerical experiments on three different problems: control-limited inverted pendulum, car-parking, and unicycle motion control and obstacle avoidance. This work is accepted for application in the IEEE Transactions on Control Systems Technology.

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MS5

Tropical Dynamic Programming for Discrete Time Stochastic Optimal Control Problems

In this talk, we consider discrete time stochastic optimal control problems with finite independent noises and Lipschitz continuous costs and dynamics. We present an iterative algorithm which approximates the value function at each time step by both max-plus and min-plus linear combinations of basic functions. If the basic functions added at each iteration are tight and valid, then we have an asymptotic convergence result. We illustrate numerically this convergence result on a toy example with linear dynamics and polyhedral costs.

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MS6

Event-Triggered Safety-Critical Control for Systems with Unknown Dynamics

Solutions to optimal control problems subject to safety-critical constraints have been shown to be obtained through a sequence of Quadratic Programs (QPs) making use of Control Barrier Functions (CBFs). A key challenge in this approach is obtaining accurate system dynamics, which is especially difficult in multi-agent systems where one agent may not have adequate data to estimate other agents dynamics. We propose to define nominal dynamics that are adaptively updated through real-time measurements and a high-order CBF that captures a safety requirement based on the nominal dynamics and error states. This leads to a sequence of QPs whose solution is triggered by specific events. We derive a condition that guarantees the satisfaction of the CBF constraint between events and illustrate how this approach works compared to the conventional time-driven approach for an adaptive cruise control problem.

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MS6

Resource-Aware Control for the Design of Accelerated Optimization Algorithms

This talk takes a dynamical systems and control approach to the design of fast optimization solvers in machine learning. Recent work in the machine learning and optimization communities seeks to shed light on the behavior of accelerated optimization methods via high-resolution differential equations. These differential equations are continuous-time counterparts of discrete-time optimization algorithms and, remarkably, their convergence properties can be characterized using the powerful tools provided by classical Lyapunov stability analysis. An outstanding open question of pivotal importance is how to discretize these continuous flows while maintaining their convergence rates. We provide an answer to this question by employing ideas from resource-aware control. The main idea is to take advantage of the Lyapunov functions employed to characterize the rate of convergence of high-resolution differential equations to design variable-stepsize discretizations that preserve by design the convergence properties of the original dynamics.

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MS6

Event-Triggered Control for Time-Varying Systems using a Positive Systems Approach

We provide new event-triggered control methods, using the notions of interval observers and positive systems. We cover time-varying linear systems, output feedback, and robustness with respect to uncertainty in the dynamics. In each case, our methods ensure global exponential stability of the closed loop system. Our illustrations include a curve tracking system from marine robotics

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MS6

Event-Triggered Control and Scheduling Co-Design

Event-triggered control plays a prominent role in current research in control and optimization, owing to its potential to reduce the computational burden as compared with traditional continuous time or zero-order hold control methods. This talk will provide an overview of recent advances in event-triggered control, including a timing model approach that co-designs controls and priority assignments to resolve contentions in networked systems, and an application to traffic management.

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MS7

Joint Optimization of Sensor Placement and Constant Luenberger Observers Gains

This paper is concerned with a sensor location problems for "optimal" state estimation based on Luenberger observers. The framework is fairly general and applies to both finite and infinite dimensional systems. We consider a general system define on a Hilbert space Z of the form

$$\dot{z}(t) = Az(t) + G\omega(t), \tag{2}$$

with measured outputs

$$y(t) = C(q)z(t) + v(t), \tag{3}$$

where $q \in Q \subseteq \mathbb{R}^d$ is a parameterization of the output operator that determines the location of the sensor and the operators $G : \mathbb{R}^m \to Z$ and $C(q) : Z \longrightarrow \mathbb{R}^p$ are Hilbert-Schmidt. Given the system above a (time independent) Luenberger observer is a linear dynamical system driven by the measured output has the form

$$\dot{z_e}(t) = Az_e(t) + F[y(t) - C(q)z_e(t)] + G\omega(t), \tag{4}$$

where $F \in \mathfrak{B}(\mathbb{R}^m, Z)$. The goal is to find F and q so that the error $e(t) = e(t, F, q) = z_e(t, F, q) - z(t)$ is "as small as possible". We employ different cost functions and formulate several optimization problems to simultaneously optimize sensor location and observer gains. Examples are given to illustrate the ideas and to compare this approach to other methods.

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MS7

Optimal Control of the 2d Evolutionary Navier-Stokes Equations with Measure Valued Controls

In this talk, we consider an optimal control problem for the two- dimensional evolutionary Navier-Stokes system. Looking for sparsity, we take controls as functions of time taking values in a space of Borel measures. The cost functional does not involve directly the control but we assume some constraints on them. We prove the well-posedness of the control problem and derive necessary and sufficient conditions for local optimality of the controls.

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MS7

Control of PDEs with Actuator Guidance Constrained over Time-Varying Reachability Sets

This work focuses on the guidance of mobile actuators employed for the control of PDEs. A practical aspect on the implementation of the actuator guidance considers the mechanical constraints of the mobile platforms carrying the actuators. Terrain platforms cannot behave as point masses without inertia; instead they must satisfy constraints which are adequately represented as path-dependent reachability sets When control algorithm commands a mobile platform to reposition itself in a different spatial location within the spatial domain, this does not occur instantaneously and for the most part the motion is not omnidirectional. This constraint is combined with a computationally feasible and suboptimal control policy with mobile actuators to arrive at a numerically viable control and guidance scheme. The control decision comes from a continuous-discrete control policy whereby the mobile actuator platform is repositioned at discrete times and dwells in a specific position for a certain time interval. Moving to a subsequent spatial location and computing its associated path over a physics-imposed time interval, a set of candidate positions and paths is derived using a path-dependent reachability set. The scheme is demonstrated with a 2D PDE having two sets of collocated actuator-sensor pairs.

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MS7

Analysis and Approximations to the Dirichlet Boundary Control of Stokes Equations

We study Dirichlet boundary control of Stokes flows in 2D polygonal domains. We consider cost functionals with two different boundary control regularization terms: the

L^2 norm and an energy space seminorm. We prove well-posedness and regularity results for both problems, develop finite element discretizations for both problems, and prove finite element error estimates. The motivation to study the energy space problem follows from our analysis: we prove that the choice of the control space $L^2(\Gamma)$ can lead to an optimal control with discontinuities at the corners, even when the domain is convex. We observe this phenomenon in numerical experiments. This behavior does not occur in Dirichlet boundary control problems for the Poisson equation on convex polygonal domains, and may not be desirable in real applications. For the energy space problem, we derive the first order optimality conditions, and show that the solution of the control problem is more regular than the solution of the problem with the $L^2(\Gamma)$ regularization. We also prove a priori error estimates for the control in the energy norm, and present several numerical experiments for both control problems on convex and nonconvex domains.

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MS8

Ergodic Linear-Quadratic Control for Systems with a Rosenblatt Noise

A control problem for an ergodic quadratic cost functional for a two dimensional system driven by a Rosenblatt process is formulated and a solution is given. Rosenblatt processes are a family of non-Gaussian processes that have a useful stochastic calculus. The noise in many physical control systems has been shown to be non-Gaussian and Rosenblatt processes seem to be a useful family of continuous non-Gaussian processes for modelling non-Gaussian noise in physical systems.

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MS8

Computable Bound for Almost Sure Convergence Rate of Ratio Consensus Algorithms

Reaching average consensus using only local communication along a network is a fundamental building block in the area of distributed computing, leading to applications such as sensor fusion and distributed optimization. Maintaining precision despite communication deficiencies is a key challenge, to tackle asynchronous message passing occurring, the concept of ratio consensus (also named push-sum) has been proposed by Kempe, Dobra, and Gehrke (2003). Besides precision for applicability one needs speed. In the current work we prove a bound on the almost sure convergence rate that is also computable for a class of ratio consensus algorithms. This extends on the works of Iutzeler, Ciblat and Hachem (2013) on similar bounds but in a more restrictive setup and conclusion, and complements the results of Gerencsr and Gerencsr (2019) identifying the exact convergence rate but providing no computable access or approximation.

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MS8

Stochastic Chemostat Models: Modeling, Long-Time Behavior, Optimal Controls, and Applications to Wastewater Treatment

In this talk, we consider the stochastic chemostat models. First, the system is formulated as a hybrid switching diffusion. Then, a complete characterization of the asymptotic behavior of the system is provided. The rate of convergence is also obtained. Moreover, we consider an application to wastewater treatment and numerical examples are given to illustrate our results. Next, controlled diffusions with a long-run average objective function are treated. The associated HamiltonJacobiBellman (HJB) equation is derived and the existence of an optimal Markov control is established. The techniques and methods of analysis in this paper can be applied to many other stochastic Kolmogorov systems.

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MS8

Distributed Filtering for Gaussian Channels with Feedback: Continuous-Time Scenarios

This paper provides a new perspective for distributed filtering based on the information-theoretic analysis of filtering problems by Mitter and Newton. We design real-time encoding strategies for Gaussian channels with feedback and provide optimality conditions for inferring states of stochastic systems.

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MS9

Bilinear Dynamic Mode Decomposition for Quantum Control

Data-driven methods for establishing quantum optimal control (QOC) using time-dependent control pulses tailored to specific quantum dynamical systems and desired control objectives are critical for many emerging quantum technologies. We develop a data-driven regression procedure, bilinear dynamic mode decomposition (biDMD), that leverages time-series measurements to establish quantum system identification for QOC. The biDMD optimization framework is a physics-informed regression that makes use of the known underlying Hamiltonian structure. Further, the biDMD can be modified to model both fast and slow sampling of control signals, the latter by way of stroboscopic sampling strategies. The biDMD method provides a flexible, interpretable, and adaptive regression framework for real-time, online implementation in quantum systems. Further, the method has strong theoretical connections to Koopman theory, which approximates nonlinear dynamics with linear operators. In comparison with many machine learning paradigms minimal data is needed to construct a biDMD model, and the model is easily updated as new data is collected. We demonstrate the efficacy and performance of the approach on a number of representative quantum systems with control.

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MS9

A Data-Driven Approach to Lifting Polynomial Systems

We study the impact of different lifting transformations, that equivalently transform a dynamical system with polynomial nonlinearity into a quadratic-bilinear (QB) system. This is performed for the computation of reduced-order models (ROMs) in the Loewner QB framework. This is a data-driven interpolation-based approach that computes a ROM whose generalized transfer functions (approximately) interpolate those of the original system. An attractive feature of the Loewner framework is that the ROM is computed using only data and does not require explicit access to the system matrices. We present different lifting formulations and their impact on the transfer functions associated with the resulting QB system. The scope is to provide guidelines for selecting lifting transformations in an automatic way; of course, this might heavily depend on the application. Although the main method of our study is the Loewner framework, the choice of lifting transformations could also be relevant for other reduced-order modeling approaches.

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MS9

Data-Driven Feedback Control Design and Stability Analysis for Complex Dynamical Systems

Recent developments in data-driven interpolatory methods has shown fantastic efficiency in model approximation, allowing to construct linear and nonlinear reduced order surrogate models based on input-output data. In this presentation, this data-driven framework is used to address (i) the linear and nonlinear controller design, and (ii) the stability analysis for applications where model description is not accessible or of infinite dimension (or not at a reasonable cost). Broad applications including both academic and industrial irrational infinite dimensional models and data collected on fluidic benchmark are used to illustrate the versatility and efficiency of the proposed method. Theoretical properties, limitations and numerical issues are also described.

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MS9

A Matrix Oriented HJB-POD Method for the Control of PDEs on a Tree Structure

The classical Dynamic Programming (DP) approach to optimal control problems is based on the characterization of the value function as the unique viscosity solution of a Hamilton-Jacobi-Bellman (HJB) equation. We will discuss a new approach for finite horizon optimal control problems where we compute the value function on a tree structure constructed directly by the time discrete dynamics and we do not use a space triangulation to solve the HJB equation. We will also apply a novel matrix-oriented reduction process (Two-sided POD-DEIM) leading to an effective, structure aware low order approximation of the original problem. Furthermore, we provide an error estimate which guarantees the convergence of the proposed method. Finally, we show the efficiency of the method through numerical tests on linear and nonlinear PDEs.

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MS10

Wasserstein Distributionally Robust Constrained Optimization: Reformulations and Consistency

This talk will focus on distributionally robust risk- and chance-constrained programs. The ambiguity set defining the distributional robustness is given as a Wasserstein neighborhood of the empirical distribution constructed from data. The first part of the talk will cover reformulations of these problems. Focussing on distributionally robust chance-constrained programs (DRCCP), we provide an exact finite-dimensional reformulation of the problem for a general class of constraint functions. We then study the convex inner approximation of the DRCCP using distributionally robust risk-constrained programs (DRRCP). We present a tractable exact reformulation of the DRRCP when the constraint function is affine in both the decision variable and the uncertainty. We then study computational strategies for solving DRRCP when the constraint function is convex or concave in the uncertainty. For the second part of the talk, we focus on asymptotic consistency of DRCCP and DRRCP. Under the assumption that the data is drawn i.i.d from an underlying distribution and that the constraint function satisfies mild technical conditions, we show that the optimal value and optimizers of the distributionally robust versions of these problems converge to the respective quantities of the original problems (defined for the underlying distribution), as the sample size increases and the radius of the ambiguity set decreases. The talk will conclude with applications of our results.

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MS10

Chance-Constrained Set Covering with Wasserstein Ambiguity

We study a generalized distributionally robust chance-constrained set covering problem (DRC) with a Wasserstein ambiguity set, where both decisions and uncertainty are binary-valued. We establish the NP-hardness of DRC and recast it as a two-stage stochastic program, which facilitates decomposition algorithms. Furthermore, we derive two families of valid inequalities. The first family targets the hypograph of a "shifted" submodular function, which is associated with each scenario of the two-stage reformulation. We show that the valid inequalities give a complete description of the convex hull of the hypograph. The second family mixes inequalities across multiple scenarios and gains further strength via lifting. Our numerical experiments demonstrate the reliability of the DRC model and the effectiveness of our proposed reformulation and valid inequalities.

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MS10

Online Learning and Optimization in Uncertain Dynamical Environments with Performance Guarantees

The ongoing development of online optimization methods is changing the way dynamical systems are characterized and controlled, focusing on online-data integration to achieve responsive system with performance guarantees under uncertainty. Examples include robotic-system learning in unknown environments and as well as online portfolio selections under extreme fluctuations in equity markets. In this talk, we discuss how our online learning and optimization frameworks were developed, by leveraging the modern measure concentration results on Wasserstein ambiguity sets. Two frameworks will be briefly outlined: 1) We focus on designing online learning algorithms that allow us to obtain high-confidence models for uncertain dynamical systems, and 2) We simultaneously learn the system while making online and optimized decisions in a quantifiably robust manner. The two frameworks are illustrated with applications to motion planning of robotic systems in various uncertain environments, and to online portfolio learning and optimization in equity markets. The proposed frameworks are unique in that they pave the way for online learning algorithms with rigorous performance bounds for control and optimization of dynamical systems, which brings a significant advancement of the state of the art.

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MS10

A General Framework for Optimal Data-Driven Optimization

We consider data-driven optimization problems where a decision-maker cannot observe the distribution of its exogenous uncertainties but rather must base its decision on a finite set of data. Recently, many such data-driven decision formulations have been considered in literature. In the face of so much choice, the question of whether some decision formulations should be preferred over others becomes pressing. We develop a general framework which allows us to compare decision formulations in terms of their statistical power. In particular, our framework allows the characterization of decision formulations which are optimal in a precise sense. Here the optimal decision formulation is characterized as the least conservative decision formulation which can guarantee that the probability of a disappointment event in which the cost of the proposed decision exceeds its predicted value decays sufficiently fast as more data becomes available. We show that under certain mild technical assumptions closely related to the existence of a sufficient statistic satisfying a large deviation principle, the optimal decision enjoys an intuitive separation into an estimation and a subsequent robust optimization step. The optimization step is robust with respect to an ambiguity set induced by the large deviation rate function of the considered estimator and is hence indirectly adapted to the underlying data-generating process.

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MS11

Deep Learning as Optimal Control and Structure Preserving Deep Learning

Over the past few years, deep learning has risen to the foreground as a topic of massive interest, mainly as a result of successes obtained in solving large-scale image processing tasks. There are multiple challenging mathematical problems involved in applying deep learning. We consider recent work of Haber and Ruthotto 2017 and Chang et al. 2018, where deep learning neural networks have been interpreted as discretisations of an optimal control problem subject to an ordinary differential equation constraint. We review the first order conditions for optimality, and the conditions ensuring optimality after discretisation. There is a growing effort to mathematically understand the structure in existing deep learning methods and to systematically design new deep learning methods to preserve certain types of structure in deep learning. Examples are invertibility, orthogonality constraints, or group equivariance, and new algorithmic frameworks based on conformal Hamiltonian systems and Riemannian manifolds. References Deep learning as optimal control problems: models and numerical methods Martin Benning, Elena Celledoni, Matthias J. Ehrhardt, Brynjulf Owren, Carola-Bibiane Schnlieb Structure preserving deep learning Elena Celledoni, Matthias J. Ehrhardt, Christian Etmann, Robert I McLachlan, Brynjulf Owren, Carola-Bibiane Schnlieb, Ferdia Sherry

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MS11

Geometric Integration of Second-Order Kinematic Vehicle Models in Route-Relative Coordinates

We propose a numerical integrator for second-order kinematic vehicle models defined in route-relative frame, often employed for decision and motion planning of au- tonomous vehicles. Under the assumption of piece-wise constant control inputs, we derive an exact spatial integrator based on simple geometric reasoning. Unlike standard numerical ODE methods, the proposed integrator has no approximation error, avoids singularities typical for route-frame integration, and is simple and efficient to implement. The method is evaluated through both open-loop simulations and optimal control through standard least-squares trajectory optimization. Based on em- pirical comparison with other integrators, we show that the developed geometric integrator is robust to edge-cases such as route-frame mapping singularities and zero velocities and also to the choice of initial guess for the optimization. This suggests that the proposed method could be a reliable choice for real-time autonomous vehicle planning and control applications.

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MS11

Geometric Numerical Integration in Simulation and Optimal Control

Studying nonlinear mechanical systems from a geometric point of view, one finds that symmetries and invariants contain valuable information on their behaviour. These structural properties play a fundamental role when designing numerical methods leading to so called structure preserving simulation tools. For example variational integrators yield symplectic-momentum conserving approximate trajectories. The benefits of structure preserving algorithms are widely accepted in forward dynamic simulations and in the numerical solution of optimal control problems using e.g. DMOCC (Discrete Mechanics and Optimal Control for Constrained Systems). On the one hand, the fidelity of the approximate solution is improved compared to standard methods by representing symmetries and invariants correctly. On the other hand, their preservation stabilises the numerical integration and thus enables coarser time grids and longterm simulation. Further, the use of symplectic integrators for the dynamics in a direct transciption method for optimal control problems leads to a special structure for the complete problem approximation.

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MS11

Reconstruction Theory: a Tool for Trajectory Generation

The connection between the dynamics in relative periodic orbits of equivariant vector fields with respect to noncompact symmetry groups, and periodic control for certain class of nonholonomic control systems on Lie groups, has promising implications and applications. We advocate the relevance, for trajectory generation problem in these type of control systems, of the qualitative properties of the dynamics in relative periodic orbits. The dynamics in relative orbits of noncompact groups can be only be of two types: either quasi-periodic, or a drift, that is the motion leave any compact subset of the relative periodic orbit as $t \to \infty$, moreover, in a given group, one of the two behaviors may be predominant, and this aspect only depends on the group. Having in mind underwater applications, we focus on the system of the hydrodynamic Chaplygin sleigh, investigating which trajectories can be obtained, at least asymptotically, by controlling some of the coordinates (shape-control variables) and using reconstruction theory from relative periodic orbits.

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MS12

Optimal Design of Graded Electrodes for Li-Ion Batteries

As Li-ion battery technology continues to mature, there is a growing need to optimise current battery designs. Doing so will improve battery power densities and lifespans without relying upon new material discovery. One recent innovation in battery design is graded electrodes which have controlled variations through the electrode thickness of the relative fractions of active particles, carbon and binder. Finding the optimal graded electrode design remains a challenge and experimental approaches have proven to be either too limited, too expensive or to take too long. To accelerate this process, this work introduces a model-driven approach to optimise graded electrode designs. The optimal designs were generated by solving a convex semi-definite programme to minimise the variation in the overpotential through the electrode thickness, with the optimised designs for Li-ion half-cells with graded $LiFePO_4$ cathodes then being built using a spray forming process. Compared to slurry-cast electrodes with the same weight fraction of active material, the optimised graded electrodes demonstrated a 44.7% increase in capacity and a 50.2% reduction in degradation rate when cycled at 1C. These results highlight the potential for model-driven approaches to efficiently and effectively optimise battery designs.

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MS12

Advanced Battery Management via Physics-Informed Machine Learning

Advanced battery management is of central importance for today's lithium-ion battery systems in ensuring their safety, performance and longevity. By nature, it is data-driven interaction with the physics of batteries. Machine learning, extending its proven success for various data understanding tasks, holds significant potential for high-performance battery modeling and control. This talk will discuss our recent journey in this emerging field. The focus will be on developing physics-aware machine learning methods to build battery models with low complexity but high predictive accuracy. We will also discuss data-based battery model identification techniques. The talk will further give an outlook the future landscape of this field by showing some potential opportunities and challenges.

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MS12

Learning and Controls for Battery Management System

With the aim of minimum time charging without damaging the cells, we propose an optimal-charging procedure based on deep reinforcement learning. In particular, we focus on a policy gradient method to cope with continuous sets of states and actions. First, we assume full state measurements from the Doyle-Fuller-Newman (DFN) model, which is projected to a lower-dimensional feature space via Principal Component Analysis. Subsequently, this assumption is removed and only output measurements are considered as the agent observations. Finally, we show the adaptability of the proposed policy to changes in the environment's parameters. The results are compared with other methodologies presented in the literature, such as the reference governor and proportional-integral-derivative approach.

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MS13

The Reduction from Ergodic to Discounted Infinite Horizon Stochastic Zero-Sum Games Problems

We consider zero-sum stochastic games with finite state and action spaces, perfect information, and mean payoff criteria. When the Markov chains associated to strategies satisfy some connectivity and acyclicity assumptions, the value of the game can be computed either by using policy iteration algorithm, or by using relative value iterations. In a previous work, we introduced a transformation of the mean-payoff problem to a discounted problem with state dependent discount rates, depending on the first hitting times of a distinguished state, which combines a Doob h-transform with a deflation technique. We shall show how this transformation allows one to transfer some recent techniques or results from the discounted framework to the ergodic one, and in particular how it allows : – to relax the conditions under which policy iterations, or value iterations can be applied; – to obtain complexity bounds for both policy and value iterations; – to apply recent techniques of variance reduced random value iterations.

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MS13

Lifting Non-Quadratic Regulator Problems to Games via Semiconvex Duality

Finite horizon linear quadratic regulator (LQR) problems represent a rare class of optimal control problems for which the associated non-stationary Hamilton-Jacobi-Bellman (HJB) partial differential equation (PDE) has an explicit solution. This explicit solution is quadratic, and its Hessian is the solution of a differential Riccati equation (DRE) with terminal data determined by the Hessian of the terminal cost. The introduction of non-quadratic cost terms, nonlinear state dynamics, or state constraints into an LQR problem destroys this quadratic structure, so that a general HJB PDE must again be solved. Such solutions are computationally expensive to obtain, often intractably so, as the numerical methods involved suffer from a curse-of-dimensionality. In this work, as a means of preserving quadratic structure, semiconvex duality is exploited to relax problematic terms in a class of non-quadratic regulator problems to yield a corresponding class of games. In these games, the two players involved select actions that correspond to the open-loop optimal controls defined in the original regulator problem, and to dual variables that select the appropriate quadratic forms that locally represent the aforementioned problematic terms. By virtue of the quadratic representations introduced, solutions of these games again involve DREs. Feedback policies for the actions of the two players are available, leading to new solution techniques for such non-quadratic regulator problems.

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MS13

Ambitropical Convexity: The Geometry of Fixed Points Sets of Shapley Operators

Shapley operators of undiscounted zero-sum two-player games are order-preserving maps that commute with the addition of a constant. The fixed points of these Shapley operators play a key role in the study of games with mean payoff: fixed points that differ, up to an additive constant, determine different optimal stationary strategies. We provide a series of characterizations of fixed point sets of Shapley operators in finite dimension (i.e., for games with a finite state space). Some of these characterizations are of a lattice theoretical nature, whereas some other rely on metric or tropical geometry. More precisely, we show that fixed point sets of Shapley operators are special instances of hyperconvex spaces: they are sup-norm nonexpansive retracts, and also lattices in the induced partial order. Moreover, they retain properties of convex sets, with a notion of "convex hull' defined only up to isomorphism. We finally study the special case of deterministic games with finite action spaces, in which these results become computational. Then, fixed point sets have a structure of polyhedral complex, encompassing both tropical polyhedra and their duals. These polyhedral complexes have a cell decomposition attached to stationary strategies of the players, in which each cell is an alcoved polyhedron of A_n type.

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MS13

Conversion of Nonlinear Second-Order Hamilton-Jacobi PDE Problems into Exact and Approximate Nonlinear First-Order Problems

A class of nonlinear, stochastic staticization control problems (including minimization problems with smooth, convex, coercive payoffs) driven by diffusion dynamics with constant diffusion coefficient is considered. The nonlinearities are addressed through stat duality. The second-order Hamilton-Jacobi partial differential equations (HJ PDE) is converted into a first-order HJ PDE in the dual variable, which contains a correction term. Approximations to the correction term will be indicated. In the subclass of cases where the nonlinearity is only in the zeroth-order term, this may be reduced to a heat equation. More generally, the new form may be converted into an HJ PDE associated to a problem where the controlled nonlinear dynamics interact with a Brownian motion only through a bilinear terminal cost, which has profound numerical implications.

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MS14

An Event-Triggered Approach to Speeding Up Parallel Computation

One of the many uses of parallel computing is to numerically solve partial differential equations. Such numerical simulations involve communication of data among the parallel processing elements. A typical implementation requires such communication at every iteration of the numerical algorithm. As the number of processors increases, the time and energy required for communication turns out to be a major portion of the overall simulation time and energy. Developing strategies to reduce communication without compromising on the quality of the solution are, thus, an important research area. In this paper, we cast the parallel numerical solution as a problem of reaching consensus in a multi-agent system. Consequently, we propose two relaxed communication schemes inspired from consensus in multi-agent systems periodic and event-triggered to reduce communication and, thus, save on simulation time and energy while guaranteeing convergence to the same solution. We model the system as a switched dynamical system and analyze properties such as stability and rate of convergence of the resulting numerical algorithm. The reduction in simulation time and communication energy due to reduced communication is shown through numerical experiments.

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MS14

On Lyapunov-Krasovskii Methods for Event-Based Control of Retarded Systems with Sampled-Data Measures, Non-Smooth Feedback, and Non-Uniform Sampling

In our 2016 SIAM Journal on Control and Optimization paper, we presented an event-based controller for nonlinear retarded systems with these features: i) only sampled-data measures of the Euclidean internal variable are needed and ii) the event function is only evaluated on sampling instants of a partition with dwell time and suitably small diameter, and involves at most a finite number of recent measures. This prior work used a function describing the feedback that needs to be Lipschitz on bounded sets, thus preventing the use of discontinuous feedbacks. This talk shows how discontinuous feedbacks can still be accommodated. We use a Lyapunov-Krasvoskii methodology, and a sampled-data event-based controller with the same features (i)-(ii). The allowed discontinuities are significant, as they include feedbacks which are discontinuous in the current internal variable. With respect to our 2021 L-CSS paper, where even more general discontinuities in the feedback are allowed at the price of only involving commensurate time delays, and of mandatory uniform sampling with suitably constrained sampling period related to delays, here these significant limitations are removed. First order interpolations of sampled-data measures are used for feedback approximation and easy implementation. It is proved that, for suitably small maximal sampling period, semi-global practical sample-and-hold asymptotic stability is guaranteed with arbitrarily small final target ball of the origin.

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MS14

Event-Triggered Control Through the Eyes of Hybrid Small-Gain Theorem

A common approach to design event-triggered controllers is emulation. The idea is to first construct a feedback law in continuous-time, which ensures the desired closed-loop properties. Then, the communication constraints between the plant and the controller are taken into account and a triggering rule is synthesized to generate the transmission instants in such a way that the properties of the continuous-time closed-loop system are preserved, and a strictly positive minimum inter-event time exists, which is essential in practice. Various triggering rules have been proposed in this context in the literature, including relative threshold, fixed threshold, dynamic triggering law to mention a few. We will show in this talk that these seemingly unrelated techniques can all be interpreted in a unified manner. Indeed, it appears that all them guarantee the satisfaction of the conditions of a hybrid small-gain theorem. This unifying perspective provides clear viewpoints on the essential differences and similarities of existing event-triggering policies. Interestingly, for all the considered laws, the small-gain condition vacuously holds in the sense that one of the interconnection gains is zero. We then exploit this fact to modify the original triggering law in such a way that the small-gain condition is no longer trivially satisfied. By doing so, we obtain redesigned strategies, which may reduce the number of transmissions as illustrated by an example.

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MS14

Event-Triggered Backstepping for Hyperbolic PDE Sandwiched Between ODEs

Motivated by vibration control of a mining cable elevator avoiding frequent actions of a massive actuator which is a hydraulic cylinder driving a head sheave, we design an event-triggered output-feedback backstepping boundary controller for coupled hyperbolic PDEs sandwiched by two ODEs, where only the measurement at the PDE actuated boundary is required. The state observer design for the overall sandwich hyperbolic PDE system, and a two-step control design including an output-feedback low-pass-filter-based backstepping boundary stabilization law and a dynamic event-triggered mechanism, are presented. The existence of a minimal dwell-time between two triggering times, and exponential convergence in the event-based closed-loop system are proved. In numerical simulations, the proposed control design is validated in the application of axial vibration control of a mining cable elevator that is 2000 meters deep, and whose dynamics include the hydraulic actuator, mining cable, and cage.

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MS15

Boundary Control for Fluid Mixing: Analysis and Computation

The question of what velocity fields effectively enhance or prevent transport and mixing, or steer a scalar field to a desired distribution, is of great interest and fundamental importance to the fluid mechanics community. In this talk, we mainly discuss the problem of optimal mixing of an inhomogeneous distribution of a scalar field via active control of the flow velocity, governed by the Stokes or the Navier-Stokes equations. Specifically, we consider that the velocity field is steered by a control input which acts tangentially on the boundary of the domain through the Navier slip boundary conditions. This is motivated by mixing within a cavity or vessel by rotating or moving walls. Our main objective is to design a Navier slip boundary control that optimizes mixing at a given final time. Non-dissipative scalars governed by the transport equation will be of our main focus in this talk. A rigorous proof of the existence of an optimal controller and the first-order necessary conditions for optimality will be derived. Computational challenges in solving the optimality conditions will be addressed. Finally, numerical experiments will be presented to demonstrate our ideas and control designs.

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MS15

Indirect Controller Design for Non-Parabolic Par-

tial Differential Equations

It can be difficult to design a controller directly for a system modelled by a partial differential equation (PDE). Approximation of the PDE using one of the many methods for obtaining a lumped approximation and then designing a controller using this approximation is a practical approach. There is now a well-established theory of approximation for controller design of parabolic PDEs. Many PDEs arise in theory and application are not parabolic. An important class of applications involve wave propagation. There are many different approximation methods for these systems that are fine for simulation. But the qualitative behaviour of the approximated eigenvalues can be quite different, depending on the numerical approximation used. This can affect controller design. Of particular interest is optimal linear quadratic control of systems that may be only asymptotically stabilizable. For linear systems, this issue only arises with infinite-dimensional systems. Sufficient conditions that guarantee when approximations to the optimal feedback result in the cost converging to the optimal cost have recently been obtained with O. Iftime and H. Zwart. Several important classes of systems, lightly damped second-order systems and a platoon-type system, have been shown to satisfy these sufficient conditions.

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MS15

In Domain Energy Shaping Control of Distributed Parameter Port-Hamiltonian Systems

In this paper we consider in-domain control of infinite dimensional port-Hamiltonian systems defined on a one dimensional spatial domain. Through an early lumping approach we extend the control by interconnection and energy shaping approach to the use of distributed control over the spatial domain. The aim is to modify the closed-loop performances over a given range of frequencies while guaranteeing the closed-loop stability of the infinite dimensional system. Two cases are investigated, the ideal case where the controller acts on the complete spatial domain (infinite dimensional distributed control), and the more realistic one where the control is piecewise homogeneous (finite rank distributed control). The proposed control strategies are illustrated through simulations on the stabilization of a vibrating Timoshenko beam.

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MS16

Nonlinear Model Predictive Control via Constraint-Aware Particle Filtering

Nonlinear model predictive control (NMPC) has gained wide use to enable various control applications. Its formulation traditionally involves repetitively solving a nonlinear constrained optimization problem online. In this talk, we examine NMPC through the lens of Bayesian estimation and highlight that the Monte Carlo sampling method offers a favorable way to implement NMPC. We develop a constraint-aware particle filtering/smoothing method and exploit it to implement NMPC. The new sampling-based NMPC algorithm allows easy and efficient execution even for complex nonlinear systems, while potentially mitigating the issues of computational complexity and local minima faced by conventional numerical optimization. We apply the proposed NMPC approach to motion planning for autonomous vehicles and illustrate its effectiveness.

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MS16

Covid-19 Multimodal Data Analysis

We have developed COVID-19 Data Archive (COVID-ARC), a platform of networked and centralized web-accessible data archives to store multimodal data related to COVID-19 and make them broadly available and accessible to the world-wide scientific community to expedite research in this area due to the urgent nature of the COVID-19 pandemic. COVID-ARC provides tools for researchers to visualize and analyze various types of data as well as a website with tools for training, announcements, virtual information sessions, and a knowledgebase wherein researchers post questions and receive answers from the community. We have performed lung and infection segmentation to generate lung masks and segmented infections to help researchers with their COVID-19 image analyses. Moreover, we have performed a variety of analyses, focusing mainly on imaging data, to identify COVID-19 positive and negative patients with high accuracy. Several examples of preliminary findings using COVID-ARC machine learning analysis as well as correlational analysis are presented.

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MS16

Ergodic Control for Linear Stochastic Differential Equations with Quadratic-Type Cost Having Indefinite Weights

In this talk, I will talk about the ergodic control for linear stochastic differential equations with quadratic-type costs having indefinite weights. We present some sufficient conditions for the finiteness and solvability of the ergodic Linear-quadratic control problem.

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MS16

Master Adjoint Systems for Risk-Sensitive Mean-Field-Type Games

Mean-Field-Type Games are games in which the payoff and or state dynamics involve not only the state-action profile but also a distribution of them. In this talk we present master adjoint systems for risk-sensitive mean-field-type games.

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MS17

Stability Analysis of Reduced Basis Model Predictive Control for Parametrized Partial Differential Equations

Model Predictive Control (MPC) is a well established approach to solve infinite horizon optimal control problems. Since optimization over an infinite time horizon is, in general, infeasible, the method determines a suboptimal feedback control by repeatedly solving finite time optimal control problems. For large-scale systems, this procedure causes immense computational effort and we thus employ the reduced basis method (RB) as a low-dimensional surrogate model. Considering a linear-quadratic optimal control problem governed by a parametrized parabolic partial differential equation, we provide a posteriori error estimators as rigorous bounds for the errors of the optimal control and the associated cost functional. Additionally, these bounds can be evaluated online efficient and can therefore be utilized to choose the length of the finite time horizon adaptively achieving provable asymptotic stability of the feedback controller of the combined RB-MPC approach. We present numerical results to validate our approach. Although we can provide rigorous results only for linear-quadratic problems, our approach may provide a guideline even for nonlinear problems.

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MS17

Near-Minimal Sensor Placement for Reconstructing States in Highly Nonlinear Sets

Sensor placement and feature selection are critical steps in engineering, modeling, and data science that share a common mathematical theme: the selected measurements should enable solution of an inverse problem. Most real-world systems of interest are nonlinear, yet the majority of available techniques for feature selection and sensor placement rely on assumptions of linearity or simple statistical models. We show that when these assumptions are violated, standard techniques can lead to costly over-sensing without guaranteeing that the desired information can be recovered from the measurements. In order to remedy these problems, we introduce a novel data-driven approach for sensor placement and feature selection for a general type of nonlinear inverse problem based on the information contained in secant vectors between data points. Using the secant-based approach, we develop three efficient greedy algorithms that each provide different types of robust, near-minimal reconstruction guarantees. We demonstrate them on two problems where linear techniques consistently fail: sensor placement to reconstruct a fluid flow formed by a complicated shock-mixing layer interaction and selecting fundamental manifold learning coordinates on a torus.

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MS17

Error Analysis of System-Theoretic Model Reduction Techniques for Bilinear Systems

In this talk, we present new results on bilinear control systems. We show under which conditions a bilinear system is asymptotically stable. Moreover, we provide a global characterization of reachability and observability in bilinear systems based on different choices of Gramians. Moreover, a new link between the output error and the $\mathcal{H}_2$-error of two bilinear systems is proved having several consequences in the field of model order reduction for such equations. It explains, e.g., why $\mathcal{H}_2$-optimal model order reduction leads to good approximations in terms of the output error. Furthermore, output errors based on the $\mathcal{H}_2$-norm can now be proved for balancing related model order reduction schemes.

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MS17

Robust Output-Feedback Stabilization for Incompressible Flows using Low-Dimensional H-Infinity Controllers

The control, in particular the stabilization, of incompressible flows using feedback controllers is of interest in practical applications and a field of ongoing research. While many output-based controller designs are known to be fragile, the standard $\mathcal{H}_\infty$-control theory provides a suitable approach to synthesize robust output-based controllers using the solution of the $\mathcal{H}_\infty$-Riccati equations. In view of stabilizing incompressible flows in simulations, two major challenges have to be addressed: the high-dimensional nature of the spatially discretized model and the structure of the differential-algebraic equations (DAEs) that comes with the incompressibility constraint. In our work, we extend the $\mathcal{H}_\infty$-balanced truncation approach and the $\mathcal{H}_\infty$-controller design to structured DAE systems, as they arise in the discretization of the Navier-Stokes equations, to construct robust low-order output-feedback controllers. Using appropriate error bounds, we can determine a priori the size of the reduced-order controller depending on the stabilization of the full-order system as well as the amount of disturbances in the discretization that needs to be handled.

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MS18

Statistical Aspects of Wasserstein Distributionally Robust Optimization Estimators

Wasserstein-based distributional robust optimization problems are formulated as min-max games in which a statistician chooses a parameter to minimize an expected loss against an adversary (say nature) that wishes to maximize the loss by choosing an appropriate probability model within a certain non-parametric class. Recently, these formulations have been studied in the context in which the non-parametric class chosen by nature is defined as a Wasserstein-distance neighborhood around the empirical measure. It turns out that by appropriately choosing the loss and the geometry of the Wasserstein distance one can recover a wide range of classical statistical estimators (including Lasso, Graphical Lasso, SVM, group Lasso, among many others). This talk studies a wide range of rich statistical quantities associated with these problems; for example, the optimal (in a certain sense) choice of the adversarial perturbation, weak convergence of natural confidence regions associated with these formulations, and asymptotic normality of the DRO estimators. (This talk is based on joint work with Y. Kang, K. Murthy, and N. Si.)

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MS18

Data-Driven Distributionally Robust Uncertainty Quantification from Dynamic Partial-State Observations

There are several control and optimization problems with dynamic random elements of an unknown distribution for which the designer seeks to make inferences using a limited amount of data. This data may only reveal partial-state information of the process, frequently also corrupted by noise. Drawing from this problem and recent advances in distributionally robust optimization we talk about how to construct Wasserstein ambiguity sets that track the evolution of dynamic probability distributions. To this end, we leverage tools from state estimation and uncertainty quantification to fuse the information from the data with the known dynamic model and provide robust uncertainty descriptions for reliable decisions. The ambiguity sets are accompanied by rigorous guarantees of containing the true distribution of the process while their construction is based on first-principles assumptions like the classes where the unknown distributions of random initial conditions, parameters, and noise elements belong.

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MS18

Learning for Control: An Inverse Optimization Approach

In data-driven inverse optimization an observer aims to learn the preferences of an agent who optimizes an unknown objective function to make decisions. Inspired by recent developments in inverse optimization, we develop a tractable learning algorithm to effectively mimic the behavior of a complex nonlinear feedback control law. The power of the proposed method is showcased in learning the popular model predictive control law. We further discuss how the control design can be robustified using the techniques from the emerging field of distributionally robust optimization. Simulation and experimental results illustrate the effectiveness of the proposed approach.

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MS18

From Moderate Deviations Theory to Distributionally Robust Optimization: Learning from Correlated Data

Given a single trajectory of correlated data generated from an unknown linear dynamical system, we study how to learn a wide class of performance functions of the underlying invariant state distribution. The function to be learned may represent, for example, an identification objective or a value function. To this end, we develop a distributionally robust estimation scheme that evaluates the worst- and best-case values of the given performance function across all stationary state distributions that are sufficiently likely to have generated the observed state trajectory. By leveraging new insights from moderate deviations theory, we prove that our estimation scheme offers consistent upper and lower confidence bounds whose exponential convergence rate can be actively controlled. In the special case of a quadratic cost, we show that the proposed confidence bounds can be characterized via the solution to Algebraic Riccati equations and as such can be computed efficiently.

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MS19

New and Surprising Perspectives on Geometric Integrators for Nonholonomic Systems

We will present a new result in nonholonomic mechanics and explore some applications to geometric integrators. Nonholonomic mechanics is not variational unlike unconstrained dynamics. However, we have recently discovered that mechanical nonholonomic systems may be seen as variational by choosing a modified Riemannian structure. In fact, its trajectories become geodesics and, in particular, they are length minimizing! We will only consider kinetic nonholonomic systems (determined by a distribution and a metric). The case of mechanical nonholonomic systems may be reduced to the kinetic case (Anahory Simoes, A.,et al:Contact bundle formulation of nonholonomic Maupertuis-Jacobi principle and a length minimizing property of nonholonomic dynamics. arXiv:2104.13178v1,2021). We will define the nonholonomic exponential map similar to its Riemannian counterpart (Anahory Simoes, A.,et al.: Radial kinetic nonholonomic trajectories are Riemannian geodesics!. arXiv:2010.12444, 2020) and a new Riemannian metric on the image submanifold of this map. In this way, we show that nonholonomic trajectories starting at q are geodesics in the new Riemannian manifold. Finally, we will discuss how one could obtain geometric integrators. We will look at two integrators arising from the theory: one uses a discretization of the nonholonomic exponential map to introduce a "Newmark-type" integrator; and another one uses the modified Riemannian metric to apply a variational integrator at each step.

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MS19

Retraction Maps: a New Seed for Geometric Integrators

The notion of retraction map is used in many research fields such as approximation of trajectories of differential equations, optimization theory, interpolation theory etc. In this talk we will review the concept of retraction map in differentiable manifolds to generalize it to obtain an extended retraction map from the tangent bundle to two copies of the configuration manifold. These new maps do not necessarily fix the initial point. We describe how to lift these extended retraction maps to the tangent and cotangent bundle which are the typical phase spaces for mechanical systems. Thus, those lifted maps are used to define geometric integrators for mechanical systems both in the Lagrangian and Hamiltonian framework.

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MS19

Sub-Riemannian Structures on Stiefel Manifolds

We reveal the geometric origins for a class of curves on Stiefel manifolds that have proved to be particularly important in solving interpolation problems arising in real applications. We show that these curves, called quasi-geodesics, are the projections of sub-Riemannian geodesics generated by certain left-invariant distributions on Lie groups that act on Stiefel manifolds. This search for the geometric characterization of quasi-geodesic curves uncovered a large class of left-invariant sub-Riemannian systems on Lie groups that turn out to admit explicit solutions with certain important properties. This will also be highlighted.

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MS19

Geometric Optimal Control and Applications to Aerospace

I will report on nonlinear optimal control theory and show how it can be used to address problems in aerospace, such as orbit transfer. The knowledge resulting from the Pontryagin maximum principle is in general insufficient for solving adequately the problem, in particular due to the difficulty of initializing the shooting method. I will show how the shooting method can be successfully combined with geometric control, allowing one to know in advance the structure of optimal trajectories ; or, with numerical homotopies, which consist of deforming continuously a problem towards a simpler one. In view of designing low-cost interplanetary space missions, optimal control can also be combined with dynamical system theory and its geometric issues, using the nice dynamical and geometric properties around Lagrange points that are of great interest for mission design.

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MS20

General Convergence Result for Continuous-Discrete Feedback Particle Filter

In this paper, we shall discuss the convergence of the continuous-discrete feedback particle filter (FPF) proposed in Yang, Blom, and Mehta (2014). The FPF is an interacting system of N particles where the interaction is designed such that the empirical distribution of the particles approximates the posterior distribution by error-based feedback control structure. Under some assumptions, it is proved that, for a class of functions ϕ, the estimate of $\phi(X_{t_n})$ by FPF converges to its optimal estimate $E[\phi(X_{t_n})|\mathscr{F}_{t_n}]$ in L^p ($\forall p \geq 2$) sense, as the number of particles goes to infinity and the numerical approximation error of computing the control input U goes to zero. Furthermore, the bound of the estimation error is also delicately analyzed.

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MS20

New Classes of Finite Dimensional Filters with Non-Maximal Rank Estimation Algebra

Ever since the Kalman filter technique was popularized, there has been an abundance of interest in finding new classes of finite dimensional recursive filters. In this work, by applying Wong's theorem about estimation algebra, we successfully construct a new class of finite dimensional filters with arbitrary state dimension n and linear rank n-2. Importantly, we show that in the new class of nonlinear filtering systems, the entries of Wong's matrix need not be constants or polynomials and can be C infinity smooth functions. This is the first time to find the non-Yau finite dimensional filters with arbitrary state dimension.

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MS23

Error Estimates for a Pointwise Tracking Optimal Control Problem of a Semilinear Elliptic Equation

We consider a pointwise tracking optimal control problem for a semilinear elliptic partial differential equation. We derive the existence of optimal solutions and obtain first order and, necessary and sufficient, second order optimality conditions. We devise two strategies of discretization to approximate the solution of the optimal control problem: a semi discrete scheme where the control variable is not discretized – the so-called variational discretization approach – and a fully discrete scheme where the control variable is discretized with piecewise constant functions. We analyze convergence properties of discretizations and derive error estimates for both solution techniques.

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MS23

Reduced Order Robust Output Regulation of Parabolic Systems

In this presentation we study robust output tracking and disturbance rejection for unstable linear parabolic partial differential equations. As our main result, we show that output tracking and disturbance rejection for our class of PDE models can be achieved using a finite-dimensional dynamic error feedback controller, and present an algorithm for construction of a low-order internal model based controller. The main novelty of the results is that all previous internal model based controller design methods have required an infinite-dimensional controller in the case of an initially unstable control system. The results are illustrated with numerical simulations of convection-diffusion equations on 1D and 2D spatial domains.

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MS23

Turnpike Property for Fractional Optimal Control Problems

We consider averages convergence as the time-horizon goes to infinity of optimal solutions of time-dependent optimal control problems to optimal solutions of the corresponding stationary optimal control problems. Control problems play a key role in engineering, economics and sciences. To be more precise, in climate sciences, often times, relevant problems are formulated in long time scales, so that, the problem of possible asymptotic behaviors when the time-horizon goes to infinity becomes natural. Assuming that the controlled dynamics under consideration are stabilizable towards a stationary solution, the following natural question arises: Do time averages of optimal controls and trajectories converge to the stationary optimal controls and states as the time-horizon goes to infinity? This question is very closely related to the so-called turnpike property that shows that, often times, the optimal trajectory joining two points that are far apart, consists in, departing from the point of origin, rapidly getting close to the steady-state (the turnpike) to stay there most of the time, to quit it only very close to the final destination and time. Here we deal with heat equations with non-zero exterior conditions associated with the fractional Laplace operator. We prove the turnpike property for the nonlocal Robin optimal control problem and the exponential turnpike property for both Dirichlet and nonlocal Robin optimal control problems.

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MS24

Stabilization of Partial Differential Equations with Disturbances

In this talk we shall discuss about the stabilization of partial differential equations subjected to disturbances. We shall review some recent results and then we shall address the stabilization of the heat equation with disturbance at the flux boundary condition, where the sign multivalued operator is used to reject the effects of the boundary disturbance.

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MS24

Feedback Stabilization of Parabolic Systems with Input Delay

This talk is devoted to the stabilization of parabolic systems with a finite-dimensional control subjected to a constant delay. Our main result shows that the Fattorini-Hautus criterion yields the existence of such a feedback control, as in the case of stabilization without delay. The proof consists in splitting the system into a finite dimensional unstable part and a stable infinite-dimensional part and to apply the Artstein transformation on the finite-dimensional system to remove the delay in the control. Using our abstract result, we can prove new results for the stabilization of parabolic systems with constant delay: the N-dimensional linear reaction-convection-diffusion equation with $N \geq 1$ and the Oseen system. We end the talk by showing that this theory can be used to stabilize nonlinear parabolic systems with input delay by proving the local feedback distributed stabilization of the Navier-Stokes system around a stationary state.

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MS24

Backstepping Control of Mixed Hyperbolic-Parabolic PDEs

In this work, we consider a class of hyperbolic-parabolic PDE system with mixed coupling terms. Compared with previous work, the coupled system we explore contains three interior-coupled terms in the domain of hyperbolic system: a coupled boundary term, an integral term, and a direct coupling term both driven by the parabolic system, which brings more challenge for controller design. Our goal is to design a boundary controller for stabilizing the whole coupled PDE system exponentially. Here, backstepping transformations are utilized to achieve the control law. Main contribution of our work is: two types of target systems are proposed and we prove they are both exponentially stable without any restrained condition; Highly coupled kernels are derived, and the well-posedness of kernels are proven by employing appropriate spaces and the infinite induction energy series without the assumption of kernels monotonicity; The invertibility of transformations are analyzed by applying the inverse transformations. Finally, numerical simulation is implemented and the results illustrate that the control laws derived from the two target system can both stabilize the mixed PDE system exponentially.

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MS24

Adaptive Boundary Observer for Linear Hyperbolic Systems Subject to Domain and Boundary Uncertainties

We are considering the problem of the state observation for a class of infinite dimensional systems modeled by the hyperbolic PDEs. The model is subject to parameter uncertainties which enter in both the domain equation and the boundary condition. An adaptive boundary observer, providing the simultaneous estimates of the system state and parameters, is designed by using the Lyapunov-based method. The exponentially convergent of the observer is guaranteed with a set of matrix inequalities. Finally, the non-equilibrium Aw-Rascle-Zhang traffic flow model is simulated to illustrate the effectiveness of the designed observer.

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MS25

Balanced Truncation for Linear and Nonlinear Truly Large-Scale Systems

Balanced truncation has been one of the most successful model reduction techniques during the past four decades. Its use in systems and control theory is ubiquitous, and it also has been adopted by many neighboring disciplines that utilize state-space modeling and transfer function concepts. Originally designed for linear (stochastic) systems, it has seen adaptations to deal with structured linear (e.g., delay, network, mechanical) systems, as well as extensions to general and structured nonlinear systems. Often, balanced truncation is perceived with the misconception that it can only be used for model order reduction of systems with a few hundred state space variables due to the high computational cost involved in computing system Gramians. In this talk, we will summarize our efforts on enabling balanced truncation to deal with truly large-scale engineering problems arising from high-fidelity modeling using, e.g., finite element methods. We will see that using enhanced numerical linear and multilinear algebra techniques, we are able to reduce linear systems with tens of millions of states, and nonlinear systems with a couple of thousands of states on desktop computers, enabling its use as building block in digital twinning and other engineering areas.

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MS25

Nonlinear Model Reduction by Moment Matching for Deterministic and Stochastic Systems

Aim of this talk is to illustrate model reduction methods for nonlinear deterministic and stochastic systems which rely on the notion of moment and to demonstrate that moments provide a powerful tool to formulate and solve complex control problems. A fundamental preliminary result for the development of model reduction by moment matching for nonlinear systems has been to recognize that the problem of determining the moments of a system corresponds to the problem of solving a particular Sylvester equation. This in turns provides an interpretation in terms of systems interconnection. Exploiting this property and this interpretation, the notion of moment has been revisited for linear systems and extended first to nonlinear systems and then in multiple directions, from time-delay to stochastic systems. In addition, the same perspective has been exploited to provide a nonlinear enhancement of the notion of phasors, to derive data-driven methods for optimal model reduction, and to develop the so-called Loewner framework for model reduction of nonlinear systems.

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MS25

Structure Preserving Discretizations of Port-Hamiltonian Distributed Parameter Systems

Many methods in scientific computing are based on generic discretizations of differential operators and disregard the underlying physical properties of the systems they simulate. In this presentation, we review a number of methods for the spatial discretization of distributed parameter systems that allow a port-Hamiltonian representation. It is shown that both the Dirac structure and the underlying energy balance of these systems can be exploited and preserved in the spatial discretization. As a consequence of the composition properties of Dirac structures, any mesh of the spatial geometry can preserve the local energy density of the system while interconnections of linked mesh elements are power preserving. It is demonstrated through a number of examples that this provides a physically meaningful approximation of the distributed parameter system.

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MS25

An Adaptive Model Order Reduction Method for Nonlinear Evolution Equations

In this work, we present an adaptive model order reduction method for parametrized nonlinear evolution equations. Precisely, we use an efficient a posteriori output error bound for constructing a reduced order model for the underlying system, so that the reduced order model is adaptively generated with a desired accuracy. Several numerical experiments are carried out to demonstrate the efficiency of the proposed adaptive model order reduction method.

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MS26

On the Neuman Bound in Rational Approximation

On the Neuman bound and the Loewner framework in rational interpolation In 1964 D.J. Newman showed that the absolute value function can be approximated by means of rational functions of degree n with an error which is less than 3 times exp(-sqrt(n)). Newmans proof was constructive. It actually turns out that his approximant is interpolatory. This leads to a connection of this circle of ideas with the Loewner framework. A few years later A.P. Bulanov improved on this bound by defining a different interpolatory approximant. In this talk we will review these and more recent results on rational approximation, discuss connections to the Loewner framework and show how interpolation points can be chosen which lead to good Loewner approximants.

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MS26

Data-Driven Prediction of Partially Observed Multiscale Systems

Complex systems with dynamics evolving on multiple timescales pose a tremendous challenge for data-driven modeling. For complex systems in oceans and climate exhibiting scale separation, the macroscopic (slow) dynamics are often modeled by treating fast variables as stochastic effects. Motivated by this idea, we use kernel methods in machine learning to approximate the Koopman evolution operator associated with the dynamical system based on only observing the slow variables. This method, called kernel analog forecasting, applies a Gaussian kernel to data points to build a Markov kernel operator and diffusion features from its eigenfunctions. Using these eigenfunctions as a basis, we construct an operator semigroup modeling the slow dynamics, and study its predictive skill on chaotic multiscale examples.

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MS26

Control Insights in Deep Neural Networks

The talk will concern Neural Ordinary Differential Equations from a control theoretical perspective to address some of the properties of Deep Neural Networks. These objectives are tackled and achieved from the perspective of the simultaneous control of systems of Neural differential equations. We will first present a strategy to achieve simultaneous control and then explain how to obtain a universal approximation theorem. Afterwards we will also present the counterparts in the context of the control of neural transport equations, enhancing the link between transport and deep neural networks.

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MS26

Context-Aware Learning of Models for Data-Driven Robust Control

Classic learn-then-stabilize approaches treat learning models of dynamical systems and computing stabilizing controllers as two separate steps. This can lead to overly conservative requirements on the accuracy of the learned models and in turn to infeasible requirements on data quality and volume in science and engineering applications. We show that if the purpose of learning models is to ultimately compute low-order stabilizing H-infinity controllers, then higher model errors can be tolerated, which lowers the sampling complexity of the learning process. In the context of H-infinity control, errors in the learned dynamical system models are compensated by a decrease in the controlled systems stability radii. This relationship between model error and stability radius allows us to quantify the amount of tolerable error. We numerically demonstrate on examples from aerospace engineering that context-aware learning of models and controllers reduces the number of samples required to stabilize dynamical systems compared to classic learn-then-stabilize approaches.

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MS27

Kernel Flows for Learning Dynamical Systems from Data

Regressing the vector field of a dynamical system from a finite number of observed states is a natural way to learn surrogate models for such systems. We present variants of the method of Kernel Flows, a variant of cross-validation, based on Maximum Mean Discrepancy and Lyapunov exponents as simple approaches for learning the kernel that appear in the emulators we use in our work.

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MS27

On the Curse of Memory in Recurrent Neural Networks: Approximation and Optimization Analysis

We study the approximation properties and optimization dynamics of recurrent neural networks (RNNs) when applied to learn input-output relationships in temporal data. We consider the simple but representative setting of using continuous-time linear RNNs to learn from data generated by linear relationships. Mathematically, the latter can be understood as a sequence of linear functionals. We prove a universal approximation theorem of such linear functionals and characterize the approximation rate. Moreover, we perform a fine-grained dynamical analysis of training linear RNNs by gradient methods. A unifying theme uncovered is the non-trivial effect of memory, a notion that can be made precise in our framework, on both approximation and optimization: when there is long term memory in the target, it takes a large number of neurons to approximate it. Moreover, the training process will suffer from slowdowns. In particular, both of these effects become exponentially more pronounced with increasing memory - a phenomenon we call the curse of memory. These analyses represent a basic step towards a concrete mathematical understanding of new phenomenons that may arise in learning temporal relationships using recurrent architectures.

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MS27

The Complexity of Neural Networks for the Approximation of Optimal Control

As demonstrated in many areas of real-life applications, neural networks have the capability of dealing with high dimensional data. In the fields of optimal control and dynamical systems, the same capability was studied and verified in many published results. Towards the goal of revealing the underlying reason why neural networks are capable of solving some high dimensional problems, we present an algebraic framework and an approximation theory for compositional functions and their neural network approximations. The theoretical foundation is developed in a way so that it supports the error analysis for not only functions as input-output relations, but also numerical algorithms. This capability is critical because it enables the analysis of approximation errors for problems for which analytic solutions are not available, such as differential equations and optimal control. We identify a set of key features of compositional functions and the relationship between the features and the complexity of neural networks. In addition to function approximations, we introduce several formulae of error upper bounds for neural networks that approximate the solutions to differential equations, optimization, and optimal control.

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MS27

Approximation, Identifiability, Controllability, Observability, and Learnability Results for Recurrent Neural Networks: A View from the 1990s

There has been much recent interest on recurrent nets, either in discrete or continuous time, which have been proposed as models for control, computation, and signal processing, and also represent limits of "deep" feedforward networks. In a control-theoretic sense, they approximate nonlinear systems on finite (or, under fading memory assumptions, infinite) time intervals, and from a computer science view point they provide universal models for digital as well as analog computation. This talk will review results from the author regarding these properties as well as learnability (in the PAC sense) and system-theoretic properties such as controllability, observability, minimality, and parameter identifiability. We'll talk about results obtained over 20 years ago, and also discuss some open problems.

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MS28

Optimal Transportation Structure of Filtering System with Correlated Noises

The feedback particle filter (FPF) is one of the important particle filter method in filtering. The FPF of noise-independent time-invariant filtering system was first proposed in 2013. After years of development, this method has been extended to high dimensions, even to the filtering problem of probability distribution of Riemannian manifolds, and the numerical method is more efficient. But the FPF of filtering system with correlated noise was proposed in 2019 by Luo. In this talk, we derive a novel optimal transportation particle filter for linear time-varying systems with correlated noises. This method can be regarded as the extension of the FPF with optimal transportation structure. However, the particles in our method are evolved in a deterministic way while we need to generate random particles in feedback particle filter. Consequently, we only need a very few particles to obtain the satisfying results and this property is especially significant for high dimensional problems. The error analysis of our method and FPF have been carried out when the system is time-invariant. Compared with feedback particle filter and ensemble Kalman filter, our method shows great efficiency in numerical experiments including both scalar case and high dimensional case.

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MS28

Feedback Particle Filter with Correlated Noises

Motivated by the mean-field game theory, the feedback particle filter (FPF) for the signal-observation nonlinear filtering (NLF) model with independent white noises, has been developed in YMM for the first time. In this talk, we shall extend this algorithm to the case where the signal process is correlated with the scalar observation process. The equation that the control inputs (K,u) satisfied has been derived by minimizing the Kullback-Leibler (K-L) divergence of the conditional density and the conditional posterior empirical distribution of the controlled particles. Then we show rigorously that the control inputs obtained is consistent, in the sense that if the initial conditional density and the empirical distribution are the same, so are the posterior ones. The explicit expression for the control input u is given if K is obtained. The numerical simulation of a scalar NLF problem with transition phenomenon has been solved by our algorithm with satisfactory performance not only in accuracy but also in efficiency.

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MS28

A Novel Real-Time Filtering Method to General Nonlinear Filtering Problem without Memory

Motivated by the supervised learning in machine learning, we develop an efficient method to numerically solve the FKE off-line. By making a temporal inverse transformation of the FKE and optimizing the loss function, the computation of the solution to the FKE is reduced to computing a linear system of equations. The proposed method has the merits of easily implementing, real-time, memoryless and more importantly applicable for moderate-high dimensional case. The efficiency of the proposed algorithm has been clearly shown by the numerical experiments.

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MS29

Reinforcement Learning for Approximate Optimal Control of Switched Systems

Decision making in adversarial environments can be complex, with the potential need to shift between different desired behaviors by an agent. Such changes in the desired behavior can be quantified by different cost functions that an agent seeks to minimize. This talk describes a reinforcement learning-based approach to approximate the optimal controller for different subsystems. Each subsystem may have varying characteristics, such as a different cost or different system dynamics. Lyapunov-based methods are developed to prove boundedness of individual subsystems and to determine a minimum dwell-time condition to ensure stability of the overall switching sequence. Uniformly ultimately bounded regulation of the states, approximation of the value function, and approximation of the optimal control policy is achieved for arbitrary switching sequences provided the minimum dwell time condition is satisfied.

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MS29

Event-Triggered Control with Resilience to Byzantine Adversaries

Event-triggered control (ETC) is an intermittent state feedback strategy motivated by advantages such as the efficient use of energy and communication bandwidth. Because communication timing conditions of ETC methods create potential vulnerabilities, resilient strategies are motivated for assured coordination in contested environments. A distributed event-triggered strategy is described for formation control and leader tracking with robustness to adversarial Byzantine agents for a class of heterogeneous multi-agent systems (MASs). A reputation-based strategy is developed for each agent to detect Byzantine agent behaviors within their neighbor set and then selectively disregard Byzantine state information. Selectively ignoring Byzantine agents results in time-varying discontinuous changes to the network topology. Nonsmooth dynamics also result from the use of the event triggered strategy enabling intermittent communication. Nonsmooth Lyapunov methods are used to analyze the developed result.

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MS31

Complementary $\mathcal{H}_2$ and $\mathcal{H}_\infty$ Filtering for Remote State Estimation with Data Dropouts

A new robust and optimal filtering design is presented first.

It is shown that this new filtering structure achieves complementary $\mathcal{H}_2$ and $\mathcal{H}_\infty$ instead of trade-off performance as demonstrated in traditional mixed $\mathcal{H}_2/\mathcal{H}_\infty$ filtering design. The simulation shows that the new filtering mechanism possesses much improved robustness while the optimal performance is well preserved. In the second part of the presentation, the new filtering scheme is applied to develop a remote estimation of state variables through unreliable communication channels characterized with data packet dropouts at no additional computational expense. Such state estimation scheme exhibits better robust and optimal performance simultaneously in terms of disturbance attenuation and transient performance than either a Kalman filter or an $\mathcal{H}_\infty$ Gaussian filter when the plant is subject to both model uncertainty and white noise. As an example, a distributed state estimation over lossy sensor networks is presented where each sensor locally constructs an estimate based on its own observation and on those collected from its neighbors.

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MS31

Dynamic Resilient Network Games for Multi-Agent Consensus under Jamming Attacks

Cyber security issues in networked multi-agent systems have gained much attention in recent years. The local nature of the agents capabilities in computation and communication leaves vulnerabilities that can be exploited by malicious attackers. In this talk, we focus on the effects of jamming attacks on the process of consensus forming by agents from a game-theoretic perspective. Specifically, we formulate a resilient network problem, which is a two-stage game where an attacker and a defender play over the connectivity of the network. The attacker attempts to disable some edges by jamming while the defender recovers them by increasing transmission power. Their utilities are based on the connectivity and the number of connected components within the graph, but the players also have constraints in the energy available for their actions. We provide full characterization of the optimal strategies for both players and then apply the game to a consensus problem, where the game is played repeatedly over time. It will be shown how different notions of connectivities affect the behaviors of the players and hence the states of the agents.

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MS31

Statistical Parameter Privacy

In this talk, we will discuss the statistical parameter privacy problem which entails privacy filter design for a sequence of sensor measurements whose joint probability density function (p.d.f.) depends on a private parameter. To ensure parameter privacy, we propose a privacy filter design framework that consists of two components: a randomizer and a nonlinear transformation. The randomizer takes the private parameter as input and randomly generates a pseudo parameter. The nonlinear mapping transforms the measurements such that the joint p.d.f. of the filter's output depends on the pseudo parameter rather than the private parameter. It also ensures that the joint p.d.f. of the filter's output belongs to the same family of distributions as that of the measurements. The design of the randomizer is formulated as an optimization problem subject to a privacy constraint, in terms of mutual information, and it is shown that the optimal randomizer is the solution of a convex optimization problem. Using information-theoretic inequalities, we show that the performance of any estimator of the private parameter, based on the output of the privacy filter, is limited by the privacy constraint. The structure of the nonlinear transformation is studied in the special cases of independent and identically distributed, Markovian, and Gauss-Markov measurements. The applications of the proposed framework in building automation and vehicular ad hoc networks will be discussed.

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MS31

Platooning with Imperfect Inter-Vehicle Communication

In the future, ordinary vehicles are expected to be automated and navigate most of the time in a self-driving mode. The potential benefits of individual automation, such as reducing fuel consumption, time efficiency, and safety, can be considerably increased if inter-vehicle communication and coordinated navigation are included. The study of platoons of vehicles that navigates together in a coordinated manner is named *platooning*, and usually considers vehicles that move in one-dimensional space since has a direct application to automated highway systems. With a proper control design, a platoon of vehicles should move coordinately, maintaining a desired speed and inter-vehicle distance, whenever is possible. But, additionally, the controller must ensure string stability, which is the property that guarantees that disturbances do not amplify along the string of vehicles, allowing scalability. String stability for platooning has been widely studied in a deterministic setup. However, a stochastic setup should be considered since, in a more realistic scenario, the inter-vehicle communication is random by nature. Indeed, inter-vehicle communication could be subject to noisy communication, random data-loss, fading, random delays, etc. In this talk, we analyze the effect that noisy communication and random data-loss may have on the string stability of a platoon of vehicles. We also discuss alternatives to reduce the effect of such non-ideal communication.

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MS32

Feedback Stabilization of the Korteweg-De Vries Equation on a Star-Shaped-Network with Internal Input Delay

In this work we deal with the exponential stability of the nonlinear Korteweg-de Vries (KdV) equation on a finite star-shaped network in the presence of delayed internal feedback. We start proving the well posedness of the system and some regularity results. Then we state an exponential stabilization result using a Lyapunov Function by imposing small initial data and a restriction over the lengths. In this part also we are able to obtain explicit expression for the rate of decay. Then we prove the exponential stability of the solutions without restrictions on the lengths and for small initial data, this result is based on an observability inequality. After that we obtain a semi-global stabilization result working directly with the nonlinear system. Next we study the case where it may happen that a control domain with delay that is outside of the control domain without delay. In that we obtain also a local exponential stabilization result. Finally we present some numerical simulations in order to illustrate the stabilization.

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MS32

Regulation of Reaction-Diffusion Equation with Boundary Control

This paper solves a regulation problem for an infinite-dimensional control system. More precisely, under the assumption that a bounded observation is given for a reaction-diffusion partial differential equation, a boundary controller is designed so that the setpoint output of the equation converges to a prescribed reference signal. This control law satisfies a finite-dimensional dynamics obtained by coupling a pole-placement control law with a converging observer. The proof of the regulation problem is based on a Lyapunov function and properties of Sturm-Liouville operators.

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MS32

PDE Backstepping Control Versus Reinforcement Learning for Traffic Flow Model

We develop reinforcement learning (RL) boundary controllers to mitigate stop-and-go traffic congestion on a freeway segment. The traffic dynamics of the freeway segment are governed by a macroscopic Aw-Rascle-Zhang (ARZ) model, consisting of 2×2 quasi-linear partial differential equations (PDEs) for traffic density and velocity. Boundary stabilization of the linearized ARZ PDE model has been solved by PDE backstepping, guaranteeing spatial L^2 norm regulation of the traffic state to uniform density and velocity. However, the stabilization result only holds locally and is sometimes affected by model uncertainty. Therefore, we reformulate the PDE boundary control problem as a RL problem that pursues stabilization without knowing the system dynamics, simply by observing the state values. The proximal policy optimization, a neural network-based policy gradient algorithm, is employed to obtain RL controllers by interacting with a numerical simulator of the ARZ PDE. The RL state-feedback boundary controllers are compared and evaluated against the rigorously stabilizing controllers in a system with perfect knowledge of the traffic flow dynamics, and then in one with only partial knowledge. We demonstrate that RL approach has learning (i.e. adaptation) potential for traffic PDE system under uncertain and changing conditions, but RL is neither simple nor a fully safe substitute for model-based control in real traffic systems.

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MS32

A Backstepping Approach to Stabilize Hyperbolic Systems: Application to a Water-Tank

We consider the so-called water tank system, modelled by shallow water equations in 1-D:

$$\begin{cases} \partial_t H + \partial_x (HV) = 0, \\ \partial_t V + V \partial_x V + g \partial_x H = -U(t), \\ V(t,0) = V(t,L) = 0, \quad \displaystyle\int_0^L H(t,x)dx = \text{cst}. \end{cases}$$

It is well-known that this system is locally controllable in $C^1([0,L])^2$ around non-uniform steady states. This also holds in Sobolev spaces, and we use this controllability result to construct exponentially stabilizing feedbacks for the linearized water-tank system around non-uniform steady states. The proof relies on the notions of system equivalence, pole-shifting, and backstepping for PDEs. This strategy of proof was already implemented to stabilize the linearized bilinear Schrdinger equation. It was adapted to the 1-D linear transport. The contrasting spectral properties of these systems lead to very different technical developments. Its success for linearized water tank shows that it can be adapted to more complex hyperbolic systems, despite the additional difficulties due to the coupling terms, and the conservation of mass.

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MS33

From Data to Reduced-Order Models via Moment Matching

A new method for data-driven interpolatory model reduction is presented in this paper. Using the so-called data informativity perspective, we define a framework that enables the computation of moments at given (possibly complex) interpolation points based on time-domain input-output data only, without explicitly identifying the high-order system. Instead, by characterizing the set of all systems explaining the data, necessary and sufficient conditions are provided under which all systems in this set share the same moment at a given interpolation point. Moreover, these conditions allow for explicitly computing these moments. Reduced-order models are then derived by employing a variation of the classical rational interpolation method. The condition to enforce moment matching model reduction with prescribed poles is also discussed as a means to obtain stable reduced-order models. An example of an electrical circuit illustrates this framework.

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MS33

Data-Driven Balancing of Linear Dynamical Systems

We present a novel reformulation of balanced truncation, a classical model reduction method. The principal innovation that we introduce comes through the use of system response data that has been either measured or computed, without reference to any prescribed realization of the original model. Data are represented by sampled values of the transfer function corresponding to the original model. We discuss parallels that our approach bears with the Loewner framework, another popular data-driven MOR method. We illustrate our approach numerically in both continuous-time and discrete-time cases.

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MS33

An Adaptive Reduced Basis ANOVA Method for High-Dimensional Bayesian Inverse Problems

In Bayesian inverse problems sampling the posterior distribution is often a challenging task when the underlying models are computationally intensive. To this end, surrogates or reduced models are often used to accelerate the computation. However, in many practical problems, the parameter of interest can be of high dimensionality, which renders standard model reduction techniques infeasible. In this work, we present an approach that employs the ANOVA decomposition method to reduce the model with respect to the unknown parameters, and the reduced basis method to reduce the model with respect to the physical parameters. Moreover, we provide an adaptive scheme within the MCMC iterations, to perform the ANOVA decomposition with respect to the posterior distribution. With numerical examples, we demonstrate that the proposed model reduction method can significantly reduce the computational cost of Bayesian inverse problems, without sacrificing much accuracy.

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MS33

Sensitivity Analysis and Error Bounds for Data-Driven Reduced-Order Models

In this contribution, we discuss novel results concerning the Loewner method for data-driven modeling and reduction of linear time-invariant systems. We study the sensitivities of eigenvalues corresponding to the Loewner pencil, which is composed of two Loewner matrices. Based on a general factorization of the Loewner pencil, a quadruple constructed directly from the data using the Loewner framework yields a model without further processing. This is verified by computing the transfer function using the generalized inverse of the resolvent. We provide a study of the sensitivity of the eigenvalues of the Loewner pencil, which are, the poles of the underlying system to be modeled. Based on an explicit generalized eigenvalue decomposition of this pencil and by making use of perturbation theory of matrix pencils, we explore two types of eigenvalue sensitivities. The first one is defined with respect to unstructured perturbations, while the second one is defined for structured perturbations. The motivation for studying these two sensitivities is that they reflect the robustness of the Loewner surrogate model. We show that the first is related to the numerical conditioning of the Loewner pencil and can be used in comparison to the pseudospectrum of the pencil. Moreover, it is shown that the second can be used to estimate eigenvalue perturbations as a result of the noise in data.

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MS34

Data-Driven Stability Analysis with the Koopman Operator

The Koopman operator offers a linear representation of nonlinear dynamical systems in terms of the evolution of observable functions. This representation is infinite-dimensional, but can be approximated through a projection onto a finite-dimensional subspace, which yields a (possibly high-dimensional) linear approximation of the nonlinear dynamics. This framework provides a systematic tool for global stability analysis, since the global stability properties of the nonlinear system can be directly inferred from the linear stability analysis of the finite-dimensional approximation. In this talk, we will leverage this approach in a data-driven context, where the linear Koopman approximation is estimated through the so-called EDMD algorithm. In particular, we will construct a candidate Lyapunov function for the linear approximation and, considering the true dynamics as a perturbation of the linear approximation, we will estimate validity bounds for the original nonlinear system. This allows to derive stability guarantees and compute an inner approximation of the attraction region in a purely data-driven fashion.

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MS34

Learning Optimal Reduced-Basis Projections for Nonlinear Systems

Reduced-order modeling techniques including balanced trunction and $\mathcal{H}_2$-optimality exploit the structure of linear dynamical systems to produce models that accurately capture the dynamics. For nonlinear systems operating far away from equilibria, on the other hand, current approaches seek low-dimensional representations of the state that often neglect small-scale features that have high dynamical significance. This leads to models with poor predictive accuracy despite being able to accurately encode and decode states. In order to improve predictive accuracy, we propose to optimize the reduced-order model to fit a collection of coarsely sampled trajectories from the original system. In particular, we optimize over the smooth manifold of biorthogonal matrices defining Petrov-Galerkin projections of the full-order governing equations. The method demonstrates significantly improved accuracy over proper orthogonal decomposition (POD)-based Galerkin projections on several fluid flow problems.

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MS34

On the Universal Transformation of Data-Driven Models to Control Systems

As in almost every other branch of science, the advances in data science and machine learning have also resulted in improved modeling and simulation of nonlinear dynamical systems. In many cases, predictive methods are advertised to ultimately be useful for control. However, the question of how to use a predictive model for control is left unanswered in most cases due to the associated challenges, namely a significantly higher system complexity, the requirement of much larger data sets and an increased and often problem-specific modeling effort. To solve these issues, we present a universal framework to transform arbitrary predictive models into control systems and use them for feedback control. The advantages are a linear increase in data requirements with respect to the control dimension, performance guarantees that rely exclusively on the accuracy of the predictive model, and only little prior knowledge requirements in control theory to solve complex control problems.

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MS34

Operator Inference and Physics-Informed Learning of Low-Dimensional Models for Incompressible Flows

Dynamical modeling of a process is essential to study its dynamical behavior and to perform engineering studies such as control and optimization. With the ease of accessibility of data, learning models directly from the data have recently drawn much attention. It is also desirable to construct compact low-dimensional models describing complex non-linear dynamics, leading to perform simulations and engineering studies on modest computer hardware. To that aim, the construction of low-order models is well reflected in the recent successes of data-driven approaches such as dynamic mode decomposition and operator inference. However, for a process, typically, there are some known physical constraints (e.g., mass conversation, energy conversation), which are not incorporated in learning models using the approaches above. In this work, we discuss the use of the operator inference approach to learning structured low-order models for incompressible flow from data. To that end, we utilize the intrinsic structure of the Navier-Stokes equations for incompressible flows and show that learning dynamics of the velocity and pressure can be decoupled, thus leading to an efficient operator inference approach for learning the underlying dynamics of incompressible flows. Finally, we show the operator inference performance in learning low-order models using some benchmark problems and compare it with an intrusive method and other data-driven approaches.

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MS35

Distributed Learning and Consensus Formation with Dynamic Networks

For a number of years now, there has been growing interest in developing algorithms for information processing and distribution, and computation in multi-agent systems, with interactions among agents taking place within neighborhoods over a network topology. Following a brief overview of this development, the presentation will focus on distributed computation and learning as it applies to consensus problems. In a typical consensus process, agents in a given group all try to agree on some quantity by communicating what they know only to their neighboring agents, dictated by an underlying network whose associated graph could be time varying, and directed or undirected. A particular type of consensus process is the so-called distributed (belief) averaging (DA), where the goal is to compute the average of some values of a quantity of interest to the agents. The talk will present several recent results (algorithms, convergence, and rates) that pertain to DA, under different scenarios, involving constraints on communication and/or information processing capabilities of neighborhood agents (such as bandwidth and compute constraints, leading to quantized iterations), or flow of private streaming data to agents. One specific application of the latter, that will be covered, is distributed on-line parametric learning in a multi-agent network, which constitutes an improved alternative to decentralized machine learning with no central agent to distribute the incoming stream of data.

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MS35

Coevolution of Opinions and Decisions in Complex Social Networks

In the past few decades, mathematical models have been widely adopted to study complex behaviors in social systems. Surprisingly, despite strong evidence of interdependence between social dynamics of opinion formation and interactive dynamics of collective decisions-making, there have been few efforts in developing a unified framework that captures the coevolution of these two dynamics on social networks. We propose a novel mathematical framework at the interface between opinion dynamics and evolutionary decision-making. Each individual, connected to the others in a network, has an opinion and can take an action. Her opinion is updated as a function of the opinions and actions of her peers. Simultaneously, she decides on the action through game-like reasoning under the social pressure to conform with others actions. We apply the proposed framework to study the introduction of an advantageous innovation. The model is able to reproduce various important real-world phenomena: the rejection of the innovation and popularity of the disadvantageous status quo, the emergence of unpopular norms, and the widespread diffusion of innovation. Analytical tools and simulations are used to prove a convergence result and elucidate the effect of the model parameters and of the network on the emergent behavior of the system.

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MS35

Nonlinear Opinion Dynamics on Networks: Consensus, Dissensus, and Tunable Sensitivity to Input

A well-defined model of opinion dynamics can be used to explain decision-making in social networks and to enable decision-making in designed networks. Such a model should exhibit fast and reliable opinion formation that rejects disturbance but responds to change without hesitancy or jitter. Since this is not possible with linear models, researchers have introduced nonlinear models. Motivated by models in engineering, biology, physics, and social science, we have derived an analytically tractable nonlinear model that exhibits the broadest range of opinion formation behaviors for an arbitrary number of agents that communicate over a network and form real-valued opinions about an arbitrary number of options. Our model can reliably (be controlled to) reach consensus or dissensus, or to switch between them, as a function of few interpretable parameters, even in fully homogeneous networks. A number of existing models are recovered as special cases of our model. Sensitivity to input is controlled through a feedback dynamic for an attention parameter that multiplies the saturated opinion exchanges. Parameters in the feedback dynamic tune implicit thresholds that govern sensitivity of the opinion formation process to input. The model provides new means for systematic study of dynamics on social and engineered networks, with applications ranging from robotic navigation and dynamic task allocation to information spread and political polarization.

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MS35

A Novel Homophily Model for Opinion Dynamics

A novel discrete time model for the evolution of the interpersonal ties in a social network is provided. In the

proposed model the state variables are the entries of the adjacency matrix of a social graph. They are binary variables that take either positive or negative values depending on whether the agents have a positive or a negative appraisal of each other. The agents update their mutual ties according to the homophily mechanism that minimizes the cognitive dissonance of the social network. At each time step all the group members compare their opinions about all the remaining agents in the network and take a deterministic decision on their mutual relationship. The model aims at emulating the dynamics of social networks in which the dynamical evolution only depends on the type of ties and not on their intensity, as it usually occurs in team supporter groups, politics, gamesThis translates into the fact that the mutual relationships only take values in the binary set $\{-1, 1\}$. Necessary and sufficient conditions for a network configuration to be an equilibrium point of the binary homophily model are formalized. A (V, Σ) factorization for the special class of matrices involved is provided, in order to give a general characterization and a social interpretation to the non-structurally balanced equilibrium points of the state space model. It allows to associate any equilibrium configuration with the structurally balanced maximal classes in the social network.

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MS36

Controllability of Hypergraphs

We develop a notion of controllability for hypergraphs via tensor algebra and polynomial control theory. Inspired by uniform hypergraphs, we propose a new tensor-based multilinear dynamical system representation, and derive a Kalman-rank-like condition to determine the minimum number of control nodes (MCN) needed to achieve controllability of even uniform hypergraphs. We present an efficient heuristic to obtain the MCN. MCN can be used as a measure of robustness, and we show that it is related to the hypergraph degree distribution in simulated examples. Finally, we use MCN to examine robustness in real biological networks.

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MS36

Optimal Control of an Epidemiological Model for Curbing the Spread of Infectious Disease

In this talk, we consider an optimal control problem formulation for curbing the spread of an infectious disease. More specifically, a SEIR (Susceptible-Exposed-Infected-Recovered) epidemiological model serves as a controlled dynamical model and the cost functional comprises of a running and terminal cost, which are functions only of the "exposed" and "infected" fractions of the total population and a perturbation term, which accounts for the effect of measurement inaccuracy on the size of the infected subpopulation. Numerical results will be presented for the above mentioned optimal control problem.

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MS36

First Order Methods for Control Synthesis

In this talk, we reexamine feedback control synthesis through the lens of first order methods in optimization. Control synthesis has historically been approached via parameterization of certificates for robustness and performance. In this talk, I will first show that first order methods facilitate a streamlined approach to directly embed data in the control synthesis process. I will then examine how such methods open up a new way of looking at some old and new problems in control. These problems include structured synthesis, indefinite least squares optimal control, and linear quadratic games. We will also discuss various geometric properties of the underlying sets for such first order methods and some of their algorithmic implications.

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MS36

Signed Control Network Curvature for Analysis of Cancer Networks-I

We study the properties of biological networks by applying analogues of fundamental concepts in Riemannian geometry and optimal mass transport theory for weighted graphs. Specifically, we employ a version of Ricci curvature for discrete spaces in order to infer robustness properties of the networks of interest. We compare three possible discrete notions of Ricci curvature (Ollivier-Ricci curvature, Bakry-Emery Ricci curvature, and Forman-Ricci curvature) on certain biological networks. While the exact relationship of each of the three definitions of curvature to one another is still not known, our network analysis based on these three notions of curvature yields very similar results. We apply the three discretizations of Ricci curvature to cancer and complementary normal networks from TCGA data for seven cancer types. All three curvatures distinguish cancer and normal networks and identify similar gene biomarkers within cancer gene interaction networks. We also compare the three Ricci curvatures to the well-known network measures betweenness centrality and clustering coefficients. Finally, we generalize Forman-Ricci curvature, which is initially defined on directed positively weighted networks, to a form that also considers the signs of the directions (e.g., activator and repressor in gene regularity networks). We call this notion the *signed-control Ricci curvature*.

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MS37

When And How Are Hybrid Dynamical Systems Conjugate To Their Classical Quotients?

In a hybrid dynamical system, the state flows until a *guard* is reached, at which point the state is *reset* so flow can continue. Identifying each state in the guard with the state it resets to defines a topological quotient—termed the *hybrifold*—onto which the hybrid systems flow descends. Our joint talk explores the smooth and topological dynamics of the hybrid system using this classical quotients flow. Near periodic orbits that pass transversely through non-overlapping guards, the hybrid systems flow is smoothly (semi)conjugate to a smooth flow on a smooth manifold. Near trajectories that pass transversely through overlapping guards in mechanical systems subject to unilateral constraints, the hybrid systems flow is piecewise-differentiable and generally *not* smoothly (semi)conjugate to a classical flow. These results motivate consideration of coarser topological methods better suited to the intrinsic non-smoothness that arises in physically-grounded hybrid models. For many such hybrid systems, topological dynamical objects correspond naturally to those of the *hybrid suspension* semiflow (related but *not* equal to the hybrifold semiflow). Moreover, Conleys fundamental theorem of dynamical systems generalizes to such hybrid systems. Mild conditions ensure that hybrid suspensions/hybrifolds are metriz*able*; additional conditions enable metriz*ation* results furnishing specific compatible metrics on these quotients.

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MS37

Brief Introduction and Overview: Categorical Characterization As a Precursor to Programming. Physical and Information Based Dynamical Systems

Many robotics problems can be modeled via a class of hybrid dynamical systems whose formalization yields a double category accounting at once for a physically relevant hybrid notion of semiconjugacy as well as hierarchical and sequential compositions. The steady state of the sequential composition is determined by that of the final constituent while its basin comprises the union of the constituents basins, thereby modeling accepted constructions of robotics. The hierarchical composition embeds a dynamical conjugate of the target dynamics upon an attracting invariant subspace of the higher dimensional host dynamics a collapse of dimension popularized by bioinspired robotics. Work in progress aims to refine the standard categorical monoidal product toward robotics methods that apply completely decoupled control modules to strongly coupled subsystems whose cross-talk can be shown to stabilize rather than disrupt the desired coordinated behavior. Systematic use of these constructions has afforded physically robust and logically well characterized robotic deployments capable of navigation and mobile manipulation amidst unexplored environments with empirical behavior surpassing in complexity and utility any of those provably correct components. Collectively, such interlocking formal and empirical developments seem like the precursors of a formal, physically grounded programming language, motivating this minisymposium.

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MS37

Geometric/Homotopical Semantics for Hybrid Dynamical Systems

Hybrid dynamical systems can often be modeled as a certain hybrid mathematical structure, a diagram of phase spaces. The diagram structure and the topologies respectively reflect discrete and continuous aspects of the dynamics. It is possible to synthesize this diagram of phase spaces into a single state space as a certain universal construction in homotopy theory called a homotopy colimit. However, passage to the homotopy colimit forgets important information about time. This talk describes an ad-hoc, but natural, refinement of the homotopy colimit as a directed space that remembers the directionality of time. Dynamical properties, such as periodicity, can then be characterized and even computed as suitable invariants on these directed homotopy colimits. With a view towards developing a higher type theory for hybrid dynamical systems, this talk then speculates on how this ad-hoc construction might be characterized as a universal construction in directed homotopy theory.

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MS37

Directed Type Theory for State Space Analysis

Type theories, which have been around in various forms for almost a century, form an important connection between computer science and mathematics. This is because of the Curry-Howard correspondence: that is to say, a type can be interpreted as a program specification to be fulfilled, as a logical proposition to be proved, or as a mathematical set (to be inhabited). Since the beginning of this century, homotopy type theory has added yet another facet to this correspondence: a type can also be interpreted as a topological space. In addition to theoretical interest, this correspondence is also of practical interest in mathematics and its applications. Since statements in type theory can be checked by a computer proof assistant (for example, by Coq or Agda), one can use this correspondence to check theorems in topology. Currently, there is much interest in extending type theory to encompass correspondences with other domains. I will talk about my development of directed homotopy type theory. This corresponds with directed homotopy theory and thus to the homotopical semantics for hybrid dynamical systems. We hope to use such a type theory then for automatically checking mathematical statements about hybrid dynamical systems. Such automatic checking is especially useful when dealing with mathematical objects, such as realistic state spaces, that are more complex than those traditionally studied by mathematicians.

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MS39

Stability Properties of a Multilayered Structure-Fluid Interactive PDE System

In this talk, we present recently derived results for a partial differential equation (PDE) system which models a fluid-structure interaction of current interest within the mathematical literature. The coupled PDE model under discussion involves a Stokes system, which evolves on a three dimensional domain, interacting with a Lamé system of elasticity which evolves on a flat portion of said fluid domain. Moreover there is an additional coupling PDE which determines the associated pressure variable of the fluid-structure system. In addition, because of the presence of an "ambient flow" vector field, the coupled PDE is not disipative.

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MS39

Optimal Control in Fluid-Structure Interactions

We are interested in minimizing the uid vorticity in the case of an elastic body moving and deforming inside the fluid, using a distributed control. This translates into analyzing an optimal control problem subject to a moving boundary fluid-structure interaction (FSI). The FSI is described by the coupling of Navier-Stokes and wave equations. The control is inherently a nonlinear control, acting as feedback on the moving frame. Its action depends on the map of the domain, which is itself dened through the dynamics of the problem. A key ingredient in the optimal control problem is represented by the long time behavior of the forced dynamics, which was an open problem in the eld. Our results include existence of solutions for all times with small distributed sources and small initial data, as well as existence of optimal control for the problem of minimization of drag in the fluid.

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MS39

Well-Posedness and Asymptotic Analysis of a Fluid-Structure Interaction Model

The model couples an internal structure (a fourth order plate) inside a fluid, with coupling at the interface between the two media. Well-posedness and asymptotic behavior are analyzed.

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MS40

The Switch Point Algorithm

The Switch Point Algorithm is a new approach for solving optimal control problems whose solutions are either singular or bang-bang or both singular and bang-bang, and which possess a finite number of jump discontinuities in an optimal control at the points in time where the solution structure changes. Problems in this class can often be reduced to an optimization over the switching points. Formulas are derived for the derivative of the objective with respect to the switch points, the initial costate, and the terminal time. All these derivatives can be computed simultaneously in just one integration of the state and costate dynamics.

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MS40

Singular Optimal Control Problems in Chemical Reactor Networks

Catalyst mixing problems in chemical reactor design have been a rich source of singular optimal control problems, with strong economic impacts and examples going back five decades. A number of examples contain many states (e.g., from discretized or reformulated PDEs), with strong nonlinearities and instabilities. This talk presents a novel bilevel nonlinear programming strategy for the singular control problem. The inner problem applies a direct transcription approach with fixed finite elements, while the outer problem adjust the finite elements to further improve the objective function and satisfy constraints on errors in the state equations and stationarity conditions of the singular problem. A challenging partial oxidation reactor optimization problem is considered, with severe instabilities due to runaway temperatures. The bilevel approach is demonstrated on this problem by finding the optimal catalyst mixing policy and significant improvement in performance.

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MS40

Optimal Control of the Fuel Allocation in a Model

for a Runner Competing in a Race

Nutrition is important when running long distance races and needs to be included in models of running strategies. We formulate a system of ordinary differential equations to represent the velocity, energy, and nutrition for a runner competing in a long-distance race. The food consumed during the race is a source term for the nutrition differential equation. In our optimal control problem, we are investigating strategies to manage the nutrition and force (source in velocity differential equation), to minimize the running time in a fixed distance race. This problem is linear in the control and involves singular components.

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MS40

Framework for Solving Bang-Bang and Singular Optimal Control Problems using Regularization and An Adaptive Radau Collocation Method

An optimization framework is described for solving bang-bang and singular optimal control problems using adaptive Legendre-Gauss-Radau collocation and control regularization. The framework consists of three stages including structure detection, structure decomposition, and domain refinement. Structure detection detects discontinuities in the control solution and analyzes the control for bang and singular arcs. After the structure is detected, the problem is decomposed into a multiple-domain formulation and transcribed using adaptive Radau collocation. The adaptive Radau collocation allows the time horizon to be partitioned into a multiple-domain setup and includes the addition of new decision variables to represent the switch times in the control profile. The last stage introduces additional constraints into the problem corresponding to each domain type. The framework is demonstrated on multiple examples, and results indicate that the method solves nonsmooth optimal control problems to a higher accuracy when compared with previously developed methods for smooth optimal control.

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MS41

Structure Preserving Balanced Model Reduction for Electrical Circuits

In this talk, we discuss how extended Gramians and balanced truncation can be exploited to reduce a linear electrical circuit model while preserving its structure. Accordingly, the reduced-order model admits a physical interpretation. Moreover, using dissipative arguments, we compute the error bound between the response of the original system and the reduced one.

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MS41

On the Matrix Equations and Matrix Inequalities in Model Order Reduction

This paper seeks to provide a retrospective study on the matrix equations and matrix inequalities involved in the prevailing model order reduction schemes. At first, Well-known Lyapunov equations, Riccati equations, Sylverster equations as well as the associated high-efficient solving algorithms are introduced. Secondly, we collect several important model order reduction problems which can only be recasted and solved in terms of linear matrix inequlities (LMI). Furthermore, we presents the new reported results on solving large-scale structured/sparse LMI.

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MS41

Clustering-Based Model Order Reduction for Water Networks

Management of large-scale water distribution networks leads to a complex optimization problem. One way to simplify this problem is to reduce the system of nonlinear differential-algebraic equations modeling the network. To reuse available network optimization software, it is beneficial to preserve the network structure in the reduced model. Clustering-based model order reduction is an approach that was proposed for structure-preserving reduction of linear multi-agent network systems. We show how this approach can be extended to water network models for a given partition. Furthermore, we propose an efficient method to finding good partitions. Finally, we demonstrate the method on a Berlin water distribution network example.

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MS41

A Method for Networks Generation with Pre-

scribed Spectrum of Laplacian Matrix

Complex real-world phenomena are often modeled as dynamical systems on networks. Moreover, dynamics in such network systems depend on the graph Laplacian and in particular on its spectrum of eigenvalues. In this paper, we focus on the problem of constructing the network structure with the pre-designed eigenvalues of a dynamical system. That is, for arbitrary pre-designed spectra, we show how to explicitly constructing such a network whose Laplacian matrix has spectrum as pre-designed. Compared with the existing network constructed methods, such as the clustering-based model reduction method, the balanced truncation model reduction method, the advantages of our proposed method are twofold:(1) a non-complete network may yield while only a complete network can be constructed with the pre-designed spectrum by using balanced truncation model reduction method;(2) our proposed constructed method also can be applied for the directed weighted networks.

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MS42

Data-Driven Reduced-Order Models via Regularized Operator Inference for a Single-Injector Combustion Process

We derive predictive reduced-order models for rocket engine combustion dynamics via Operator Inference, a scientific machine learning approach that blends data-driven learning with physics-based modeling. The non-intrusive nature of the approach enables variable transformations that expose system structure. We advance the formulation robustness and algorithmic scalability of the Operator Inference approach by formally introducing regularization to avoid over-fitting. The task of determining an optimal regularization is posed as an optimization problem that balances training error and stability of long-time integration dynamics. A scalable algorithm and open-source implementation are presented, then demonstrated for a single-injector rocket combustion example. This example exhibits rich dynamics that are difficult to capture with state-of-the-art reduced models. With appropriate regularization and an informed selection of learning variables, the reduced-order models exhibit high accuracy in re-predicting the training regime and acceptable accuracy in predicting future dynamics, while achieving close to a million times speedup in computational cost. When compared to a state-of-the-art model reduction method, the Operator Inference models provide the same or better accuracy at approximately one thousandth of the computational cost.

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MS42

Accelerated Maximum Likelihood Estimation of States and Parameters in Power Grids using Clustering

In this presentation, we discuss maximum likelihood estimation (MLE) of states and parameters in power grids, based on first-principles models involving stochastic differential-algebraic equations. State and parameter estimation is essential for enhancing power grid resilience in the presence of fluctuating energy consumption and production. Stochastic first-principles models combine knowledge of the key phenomena in the system (conservation of energy, Kirchhoff's laws, etc.) with knowledge of the uncertainty in parameters, inputs, or other model quantities. Furthermore, based on the maximum likelihood estimates, the Cramr-Rao bound provides confidence intervals on the parameters, and the goodness-of-fit of the model can be assessed using the likelihood ratio test. Such information is useful in the design of experiments, e.g., in choosing the number and placement of sensors or frequency of measurements. As power grid models are nonlinear, we use linearization to approximate the nonlinear transformations of the stochastic variables and evaluate the likelihood function which is maximized in MLE (essentially, we use the continuous-discrete extended Kalman filter for this purpose). MLE involving these approximations is computationally demanding. Therefore, we present a clustering approach for reducing the power grid models, and we demonstrate that the reduced model can be used in the design of experiments, e.g., in choosing the frequency of observations.

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MS42

Closed-Loop Controller Synthesis for Mixed Data and First-Principle Models

In complex applications, a model description in terms of differential equations, which accurately represent the real-world phenomenon's dynamics, may not be available. Instead, the actual dynamics may be decomposed into modeled and unmodeled components. If data of the unmodeled components is available, then machine learning can be used to enrich the first-principle model with a purely data-driven model. In this talk, we discuss the challenges that come with such a mixed model and present a novel method to synthesize a controller such that the closed-loop system is passive. The methodology uses the port-Hamiltonian system formulation in combination with the small-gain theorem. The theoretical findings are illustrated with a numerical example.

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MS42

Funnel-MPC: a Data-Driven MPC Paradigm

Model Predictive Control (MPC) is nowadays a widely used control technique for linear and nonlinear systems due to its ability to handle multi-input multi-output systems under control and state constraints. However, for the usage of MPC initial and recursive feasibility have to be ensured. Furthermore, it is inherently necessary to have a sufficiently accurate model to predict the system behavior and compute an optimal control signal. Complementary, funnel control is an adaptive high-gain output-error feedback. Under certain structural assumptions this concept guarantees the tracking of a prescribed reference signal within predetermined bounds. In this talk we propose the new concept Funnel-MPC, which combines both concepts, i.e. MPC and funnel control. During an initial learning phase the model-free funnel control guarantees that the imposed constrains are met. Afterwards, the advantages of the model-based MPC scheme are exploited. To this end, funnel-inspired stage costs are used, for which initial and recursive feasibility can be rigorously shown.

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MS43

A Biased Assimilation Model in Presence of Antagonism

A biased assimilation model of opinion dynamics is a nonlinear model in which opinions exchanged in a social network are multiplied by a state dependent term having the bias as exponent, and expressing the bias of the agents towards their own opinions. The aim of this work is to extend the bias assimilation model to signed social networks. We show that while for structurally balanced networks polarization to an extreme value of the opinion domain (the unit hypercube) always occurs regardless of the value of the bias, for structurally unbalanced networks a stable state of indecision (corresponding to the centroid of the opinion domain) also appears, at least for small values of the bias. When the bias grows and passes a critical threshold which depends on the amount of 'disorder' encoded in the signed graph, then a bifurcation occurs and opinions become again polarized.

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MS43

Social Influence and Opinion Dynamics from Expertise and Confidence

In this work, we study interpersonal influence in small groups of individuals who collectively execute a sequence of intellective tasks. We observe that along an issue sequence with feedback, individuals with higher expertise and social confidence are accorded higher interpersonal influence. We also observe that low-performing individuals tend to underestimate their high-performing teammate's expertise. Based on these observations, we introduce three hypotheses and present empirical and theoretical support for their validity. We report empirical evidence on longstanding theories of transactive memory systems, social comparison, and confidence heuristics on the origins of social influence. We propose a cognitive dynamical model inspired by these theories to describe the process by which individuals adjust interpersonal influences over time. We demonstrate the model's accuracy in predicting individuals' influence and provide analytical results on its asymptotic behavior for the case with identically performing individuals. This presentation includes the results obtained in [O. Askarisichani, E. Y. Huang, K. S. Sato, N. E. Friedkin, F. Bullo, and A. K. Singh. Expertise and confidence explain how social influence evolves along intellective tasks. http://arxiv.org/abs/2011.07168].

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MS43

Opinion Dynamics and Social Instabilities: the Roles of Zealots, Homophily and Ranking

Why do people change their minds and what are the consequences? This talk will discuss several models which use approaches from statistical physics and dynamical systems to analyze opinion dynamics in social systems. In particular we show the splintering role of zealots, how homophily which is meant to increase social cohesion can actually impede global consensus, and how the balance of talent and social reputation can cause cascading rank rearrangements in established social hierarchies.

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MS43

Modelling Expressed and Private Opinion Forma-

tion in Social Influence Networks

Mathematical models of opinion formation on social networks originate from seminal works of French and Harary (1950s), and DeGroot (1970s). Subsequent advances have enabled models to capture a range of social phenomena, such as a group of individuals converging to a consensus, reaching a persistent disagreement, or becoming polarised. However, almost all models assume that individuals always share their true opinions, despite a wealth of social psychology literature indicating that in many social scenarios, an individual may express an opinion that is different from his/her true one. In this talk, we propose a model in which each individual has both a private (true) opinion and an expressed opinion that he/she shares with others in the network. For each individual, the two opinions co-evolve in an interdependent manner. We prove a general convergence result, and show that under generic conditions, a discrepancy arises between the steady state expressed and private opinion of each individual. The model is then used to revisit two classical social psychology phenomena. First, we revisit Aschs seminal conformity experiments from the 1950s, showing how all observed outcomes of the experiments can be recovered from intuitively reasonable model parameter values. Then, we show how a few extremist zealots can create pluralistic ignorance, whereby the majority of individuals privately support one position, while assuming there is a majority support for a different position.

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MS44

Low-Dimensional Dynamics of Morphogenetic Patterning

During early Drosophila embryogenesis, a network of gene regulatory interactions orchestrates terminal patterning, playing a critical role in the subsequent formation of the gut. We used the MS2/MCP mRNA labeling system and light sheet microscopy to monitor the individual components of this network across 90 minutes prior to gastrulation. We developed a computational approach for fusing imaging datasets of the individual components into a common multivariable trajectory. We will discuss details, advantages, and statistical and conceptual limitations of our heterogeneous data fusion approach and demonstrate how it reveals low intrinsic dimensionality of posterior patterning and cell fate specification. High conservation of the network in question suggests that our results could provide insight into mechanisms of gene regulation during development of other species. The presented data fusion strategy is the first step towards our overarching aim of establishing a unified framework that would allow to explore how stochastic spatiotemporal signals give rise to highly reproducible morphogenetic processes.

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MS44

Moment-Based Methods for Data-Enabled Inference and Control of Dynamic Populations

In many cutting-edge applications involving large dynamic population systems, such as neuronal networks, robot swarms, quantum spin ensembles, and cellular oscillators, placing dedicated sensors to monitor the time-evolution of the states of individual systems in a population is infeasible. However, aggregated type of spatially sparse measurements, such as coarse or fragmented images and partial snapshots, can be obtained. The availability of such aggregated measurements opens up the possibility for utilizing population-level observation and feedback to learn system dynamics and to close the loop in ensemble control systems. In this talk, we will introduce a moment-based framework that utilizes the idea of statistical moments induced by aggregated measurements to synthesize a novel approach for learning, analysis, and control of ensemble systems. In particular, we will cast ensemble control problems as the classical moment problem and present the dynamic connection between ensemble systems and their moment systems, by which the control-theoretic analysis, e.g., controllability, and design can be carried over through the study of the moment system. Moreover, we will illustrate how the proposed moment-based method enables a purely data-driven architecture to infer ensemble systems with unknown dynamics and close the loop via designing moment-dependent feedback laws for ensemble control systems.

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MS44

Robustness of Networked Systems to Unintended Interactions with Application to Engineered Genetic Circuits

In a networked dynamical system, subsystems are interconnected through prescribed interactions to achieve a desired emergent behavior. In many applications, one subsystem can also affect others through "unintended" interactions that change the emergent network's behavior. Although unintended interactions can be modeled as disturbance inputs to the subsystems, these disturbances depend on the network's states. Therefore, a disturbance attenuation property of each isolated subsystem is, alone, insufficient to guarantee that the network behavior is robust to unintended interactions. In this talk, I will provide sufficient conditions on subsystem dynamics and interaction maps, such that the network's behavior is robust to unintended interactions. These conditions require that each subsystem attenuates external disturbances, is "near-monotone", the unintended interaction map is monotone, and the prescribed interaction map does not contain feedback loops. We apply these conditions to design decentralized biomolecular controllers in resource-limited genetic circuits to ensure that a prescribed network behavior is achieved despite unintended coupling due to resource sharing. More generally, our results provide conditions under which robustness of constituent subsystems is sufficient to guarantee robustness of a network to unintended interactions.

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MS44

Hypergraph Dissimilarity Measures

In this work we present a novel mathematical framework for hypergraph comparison. Hypergraphs are generalizations of graphs in which edges may connect any number of vertices, thereby representing multi-way relationships which are ubiquitous in many real world networks including neuroscience, cyber security, social networks, and bioinformatics. We propose two approaches for hypergraph comparison. The first approach is based on transforming the hypergraph into a graph representation and then invoking the standard graph dissimilarity measures. The second approach relies on mathematical representations which intrinsically capture multi-way relations using tensor or higher-order hypergraph walks based methods. Within each approach we present a collection of measures which either assess hypergraph similarity at a specific scale e.g. local, mesoscopic or global, or provide a more holistic multi-scale comparison. We test these measures on synthetic networks to assess their usability and develop a guide for the selection of an appropriate one depending on the application. Finally, we apply the methods to real-world biological datasets.

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MS45

Programming Physical Systems with Linear Dependent Type Theory

Linear dependent type theory would be an essential feature of a quantum programming language, if quantum resources and classical control were to be integrated. Proto-Quipper is a family of functional programming languages for describing quantum circuits that are susceptible of semantics and other formal foundations. Recent work presented categorical and operational semantics of linear dependent type theory, and thereby integrated (a version of) Proto-Quipper with dependent types. In fact, this formalism is flexible enough to apply to not only quantum programming but also any linear type theory that integrates linear resources and non-linear parameters. We therefore conjecture that it provides a new programming-language approach to various systems that can be described by monoidal categories, one example being the hybrid dynamical compositions of robotics.

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MS45

Embedding Linear Temporal Logic into Hybrid Dynamical Type Theories

Linear-time temporal logic (LTL) is the state-of-the-art language for specifying high-level behavioral invariants in many safety-critical settings. In robotics, the dominant implementation paradigm has been to translate an LTL specification into a discrete automaton which, in turn, is translated into a hybrid controller. We present an alternative bottom-up approach based on linear logic, the internal language of symmetric monoidal categories. Leveraging recent work on categories of hybrid systems, we develop linear type theories for mobile manipulation where the atomic types are presheaves on a category of physically-grounded hybrid systems. We then embed a useful fragment of LTL into these hybrid dynamical type theories, enabling correct-by-construction programming of hybrid controllers.

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MS45

Programming Robotic Tasks in Linear Temporal Logic

In thistalk, I willpresent a new reactive temporal logic planning algorithm for multiple robots that operate in environments with unknown structure. The robots are equipped with individual sensors that allow them to continuously learn a map of the unknown environment. The goal of the robots is to accomplish complex collaborative tasks expressed using Linear Temporal Logic (LTL) formulas. The majority of existing LTL planning approaches rely on discrete abstractions of the robot dynamics operating in known environments and, as a result, they cannot be applied to the more realistic scenarios where the environment is initially unknown. We address this novel challenge by proposing the first reactive and abstraction-free LTL planning algorithm that can be applied for complex mission planning of multiple robots operating in unknown environments. The proposed algorithm is complete under mild assumptions on the structure of the environment and the sensor models. I will present numerical simulations and hardware experiments that illustrate the theoretical analysis and show that the proposed algorithm can address complex real-world planning tasks for large-scale multi-robot systems in unknown environments.

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MS45

Double-Categorical Semantics of Gradual Typing

Double categories have recently been used to model composition of hybrid systems. Recently, in the field of programming languages, we have shown that the structure of a logical relation for gradual typing exhibits the algebraic structure of a double category, analogous to the relationship between parametricity and reflexive graph categories. To study gradual typing axiomatically, we have developed gradual type theory, a sound and complete formal syntax for vertically thin double categories. In the talk, we will give an introduction to double categories and discuss how we might generalize gradual type theory to model arbitrary double categories.

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MS46

Regularization with the Total (Generalized) Variation of the Normal using ADMM/Split-Bregman

The total variation of the normal vector as a regularizer for geometric inverse problems is formulated. The normal vector is thereby explicitly treated as an element of the unit sphere. Such non-smooth shape optimization problems can be solved via a suitable Split Bregman approach (ADMM) on a triangular discretization. Naturally, the TV regularizer suffers from staircasing, which yields piecewise planar reconstructions. Therefore an extension that originated in imaging, the total generalized variation, is formulated for manifold-valued data on discrete surfaces. Numerical experiments are presented for mesh denoising and inpainting problems.

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MS46

The Strip Method for Shape Derivatives

A major challenge in shape optimization is the coupling of finite element method (FEM) codes in a way that facilitates efficient computation of shape derivatives. This is particularly difficult with multiphysics problems involving legacy codes, where the costs of implementing and maintaining shape derivative capabilities are prohibitive. The volume and boundary methods are two approaches to computing shape derivatives. Each has a major drawback: the boundary method is less accurate, while the volume method is more invasive to the FEM code. We introduce the strip method, which computes shape derivatives on a strip adjacent to the boundary. The strip method makes code coupling simple. Like the boundary method, it queries the state and adjoint solutions at quadrature nodes, but requires no knowledge of the FEM code implementations. At the same time, it exhibits the higher accuracy of the volume method. As an added benefit, its computational complexity is comparable to that of the boundary method, i.e., it is faster than the volume method. We illustrate the benefits of the strip method with numerical examples.

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MS46

On Pre-Shape Calculus

Deformations of the computational mesh arising from optimization routines usually lead to decrease of mesh quality or even destruction of the mesh. We propose a theoretical framework using pre-shapes to generalize classical shape optimization and -calculus. We define pre-shape derivatives and derive according structure and calculus theorems. In particular, tangential directions are featured in pre-shape derivatives, in contrast to classical shape derivatives featuring only normal directions. Techniques from classical shape optimization and -calculus are shown to carry over to this framework. An optimization problem class for mesh quality is introduced, which is solvable by use of pre- shape derivatives. This class allows for simultaneous optimization of classical shape objectives and mesh quality without deteriorating the classical shape optimization solution. The new techniques are implemented and numerically tested for 2D and 3D.

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MS46

Shape Optimization Mitigating Coastal Erosion

Coastal Erosion describes the displacement of land caused by destructive sea waves, currents or tides. Major efforts have been made to mitigate these effects using groins, breakwaters and various other structures. We try to address this problem by applying shape optimization techniques on the obstacles. We model the propagation of waves towards the coastline, using Shallow Water Equations. The obstacle's shape is optimized over an appropriate cost function to minimize the energy of water waves along the shore, without relying on a finite-dimensional design space, but based on shape calculus.

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MS47

The Relativistic Euler Equations with a Physical Vacuum Boundary

We consider the relativistic Euler equations with a physical vacuum boundary and an equation of state $p(\varrho) = \varrho^\gamma$, $\gamma > 1$. We establish the following results. (i) local well-posedness in the Hadamard sense, i.e., local existence, uniqueness, and continuous dependence on the data; (ii) low regularity solutions: our uniqueness result holds at the level of Lipschitz velocity and density, while our rough solutions, obtained as unique limits of smooth solutions, have regularity only a half derivative above scaling; (iii) stability: our uniqueness in fact follows from a more general result, namely, we show that a certain nonlinear functional that tracks the distance between two solutions (in part by measuring the distance between their respective boundaries) is propagated by the ow; (iv) we establish sharp, essentially scale invariant energy estimates for solutions; (v) a sharp continuation criterion, at the level of scaling, showing that solutions can be continued as long as the velocity is in $L^1_t Lip_x$ and a suitable weighted version of the density is at the same regularity level. This is joint work with Mihaela Ifrim and Daniel Tataru.

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MS47

Null Controllability of Some Free-Boundary Problems

This talk is concerned with the null controllability of several free-boundary problems. Among them, we will consider the one-phase and two-phase Stefan problems with distributed or boundary controls. We will prove some local results. More precisely, it will be shown that there exist controls such that an associated dependent variable (resp. an associated interface) is steered to zero (resp. to a prescribed location) provided the initial data and interface position are sufficiently close to the targets. We will also present some numerical methods for the computation of null controls and will illustrate the techniques with several numerical experiments.

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MS47

Stationary Variational Problems with Distributional Gradient Constraints

We consider nondiffusive variational problems with mixed boundary conditions and (distributional and weak) gradient constraints. The upper bound in the constraint is either a function or a Borel measure, leading to the state space being a Sobolev one or the space of functions of bounded variation. We address existence and uniqueness of the model under low regularity assumptions, and rigorously identify its Fenchel pre-dual problem. The latter in some cases is posed on a non-standard space of Borel measures with square integrable divergences. We also establish existence and uniqueness of solution to this pre-dual problem under some assumptions. We finalize the talk with numerical tests.

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IP1

Welcome Remarks and Presentation: On Some Connections Between Combinatorics, Computational Complexity and the Physics of Phase Transition

We illustrate the connections in question on an example of counting matchings (also known as monomer-dimer configurations) in graphs. It turns out that the total number of matchings in a given graph is determined within any prescribed relative error by the numbers of matchings of a rather small size, roughly proportional to the product of the square root of the largest degree of a vertex and the logarithm of the number of vertices of the graph. This, in turn, leads to an efficient deterministic algorithm for approximate counting of matchings. The result follows from the Heilmann - Lieb Theorem on the roots of the matching polynomial of a graph, interpreted in statistical physics as the absence of phase transition in monomer-dimer systems. We will discuss a possibility to bypass the phase transition obstruction in counting algorithms by using complex temperatures.

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IP2

Recent Advances in Ramsey Theory

Ramsey theory studies the paradigm that every sufficiently large system contains a well-structured subsystem. Within graph theory, this translates to the following statement: for every positive integer s, there exists a positive integer n so that for every partition of the edges of the complete graph on n vertices into two classes, one of the classes must contain a complete subgraph on s vertices. Beginning with the foundational work of Ramsey in 1928, the main question in the area is to determine the smallest n that satisfies this property. For many decades, randomness has proved to be the central idea used to address this question. Very recently, we proved a theorem which suggests that "pseudorandomness and not complete randomness may in fact be a more important concept in this area. This new connection opens the possibility to use tools from algebra, geometry, and number theory to address the most fundamental questions in Ramsey theory. This is joint work with Jacques Verstraete.

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IP3

Longest Common Subsequences

Given two words, one way to measure their similarity is to look for a longest common subsequence (LCS). The LCS is commonly used in applications such as bioinformatics and coding theory. In this talk we describe several extremal and probabilistic problems related to the LCS. Various parts of the talk are based on works with Chris Cox, Zichao Dong, Venkatesan Guruswami, Johan Hstad, Raymond Hogenson, Jie Ma, and Lidong Zhou.

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IP4

The Log-rank Conjecture

The log-rank conjecture is one of the tantalizing open problems in communication complexity. Initiated by Lovasz and Saks in 1988, it speculates that any binary matrix of low rank can be partitioned into a small number of monochromatic rectangles. Despite over 30 years of research, we are still very far from resolving it. In this talk, I will describe recent progress on the log-rank conjecture. In particular, I will discuss progress on special cases, which has surprising connections to the analysis of boolean functions; and a refutation of an extension of the log-rank conjecture to randomized communication.

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IP5

Centrally Symmetric Neighborliness: Polytopes vs Spheres

A centrally symmetric simplicial complex is called cs-k-neighborly if every k of its vertices no two of which are antipodal form a face. How neighborly can a centrally symmetric polytope be as a function of its dimension and the number of vertices? How neighborly can a centrally symmetric sphere be? Are there centrally symmetric analogs of the cyclic polytope? The motivation for studying these questions stems from the desire to find tight upper bounds on the face numbers of various classes of simplicial complexes as well as from the surprising connections between cs-neighborliness and the seemingly unrelated areas of error-correcting codes and sparse signal reconstruction. In the talk I will survey many fascinating developments in this subject including some very recent results joint with Hailun Zheng.

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IP6

List-decodability of Random Ensembles of Codes

Given a set C of binary vectors, how many points of C lie in any Hamming ball of a fixed radius? This is the (combinatorial version of the) list-decoding question in error correcting codes. List-decoding is a classical notion in error correcting codes, and has applications from communication to complexity theory. In this talk, I'll discuss recent progress on the list-decodability of structured random ensembles of codes. For example, what happens if C is a random subspace of $GF(2)^n$? Or the kernel of a random sparse matrix? Or a Reed-Solomon code with random evaluation points?

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IP7

Large Deviations in Random Graphs

Suppose that $Y_1, \ldots, Y_N$ are i.i.d. (independent identically distributed) random variables and let $X = Y_1 + \ldots + Y_N$. The classical theory of large deviations allows one to accurately estimate the probability of the tail events $X < (1-c)E[X]$ and $X > (1+c)E[X]$ for any positive c. However, the methods involved strongly rely on the fact that X is a linear function of the independent variables $Y_1, \ldots, Y_N$. There has been considerable interestboth theoretical and practicalin developing tools for estimating such tail probabilities also when X is a nonlinear function of the Y_i. One archetypal example studied by both the combinatorics and the probability communities is when X is the number of triangles in the binomial random graph $\mathrm{G}(n,p)$. I will discuss recent developments in the study of the tail probabilities of this random variable. The talk is based on joint works with Matan Harel and Frank Mousset and with Gady Kozma.

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IP8

Presentation and Closing Remarks: Local Computation Algorithms

Consider a setting in which inputs to and outputs from a computational problem are so large, that there is not time to read them in their entirety. However, if one is only interested in small parts of the output at any given time, is it really necessary to solve the entire computational problem? Is it even necessary to view the whole input? We survey recent work in the model of "local computation algorithms" which for a given input, supports queries by a user to values of specified bits of a legal output. The goal is to design local computation algorithms in such a way that very little of the input needs to be seen in order to determine the value of any single bit of the output. Though this model describes sequential computations, techniques from local distributed algorithms have been extremely important in designing efficient local computation algorithms. In this talk, we describe results on a variety of problems for which sublinear time and space local computation algorithms have been developed – we will give special focus to finding maximal independent sets and generating random objects.

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SP1

2020 Dnes Knig Prize Lecture: Ramsey Graphs

An n-vertex graph is called C-Ramsey if it has no clique or independent set of size C log n. All known constructions of Ramsey graphs involve randomness in an essential way, and there is a line of research towards showing that in fact all Ramsey graphs must obey certain richness properties characteristic of random graphs. I will survey the history of this area, and discuss the resolution of an old conjecture posed by Erdos, Faudree and Ss, which was joint work with Benny Sudakov. I will also discuss some new directions joint with Lisa Sauermann.

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JP1

Joint Plenary with SIAM Annual Meeting AN21: Stability in Strategic Queueing Systems

Over the last two decades we have developed good understanding how to quantify the impact of strategic user behavior on outcomes in many games (including traffic routing and online auctions), and showed that the resulting bounds extend to repeated games assuming players use a form of no-regret learning to adapt to the environment. Unfortunately, these results do not apply when outcomes in one round effect the game in the future, as is the case in many applications. In this talk, we study this phenomenon in the context of a game modeling queuing systems: routers compete for servers, where packets that do not get served need to be resent, resulting in a system where the number of packets at each round depends on the success of the routers in the previous rounds. In joint work with Jason Gaitonde, we analyze the resulting highly dependent random process. We find that if the capacity of the servers is high enough to allow a centralized and knowledgeable scheduler to get all packets served even with double the packet arrival rate, then despite selfish behavior of the queues, the expected number of packets in the queues will remain bounded throughout time, assuming older packets have priority. Further, if queues are more patient in evaluating their outcomes , maximizing their long-run success rate, stability can be ensured with just 1.58 times extra capacity, strictly better than what is possible assuming the no-regret property.

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CP1

Random Embeddings of Random Regular Graphs

Using the well-known correspondance between the maps of a graph and the sets of assignments of cyclic rotations to the boundary of each of its vertices, one may endow the ensemble of maps of a given graph with the uniform probability distribution and consider the number of faces in a random map as a random variable. In 1990, Saul Stahl conjectured that for almost all graphs G the expected number of faces in a random map of G is close to the natural logarithm of its number of edges. This talk will present a positive solution to this conjecture for regular graphs. In particular, we show that the expected number of faces in a random map of a random d-regular multigraph on n vertices is $\Theta(\log(dn))$, where d can be any function of n. We then build upon this result to show that, if d is fixed while n grows arbitrarily large, the expected number of faces in a random map of a random d-regular simple graph is $\Theta(n)$. This is joint work with Jesse Campion Loth, Tom Masark, Bojan Mohar, and Robert mal.

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CP1
Phase Transition of Epidemic Contact Processes on Networks

COVID-19 has a considerable effect on public health and the global economy. Mathematical modeling of contact process on networks plays a vital part in predicting and controlling the ongoing pandemic. In this proposal, we will be interested in the general susceptible-infected susceptible (SIS) epidemic model, where each site of the network is either infected or healthy (but susceptible). An infected site becomes healthy at rate 1 independent of other sites and is again susceptible to the disease, while a susceptible site becomes infected at a rate λ times the number of its infected neighbors. The first task of the proposal will analyze the phase transition of epidemics reconstructability on general Galton-Watson trees, where each individual of a given generation on the tree gives birth to a random number of children in the next generation, and infection and recovery events in the process happen independently from vertex to vertex with mutations. Usually real-world networks are quite large, and every vertex from the network plays the different role, leading to a inhomogeneous random graph. Therefore, our second purpose is to establish the necessary and sufficient criterion of the phase transition on the random graph with only a uniformly random vertex in the graph infected initially while all the other ones healthy. This project has wide applications in understanding the propagation of a disease, predicting the future extension of the outbreak, etc.

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CP1
Orthogonal Colourings of Random Geometric Graphs

Two colourings of a graph are orthogonal if they have the property that when two vertices receive the same colour in one colouring, then those vertices must receive distinct colours in the other colouring. In this talk, orthogonal colourings of random geometric graphs are studied. First, it is shown that sparse random geometric graphs have optimal orthogonal colourings. Then, an upper bound on the orthogonal chromatic number for dense random geometric graphs is obtained.

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CP1
On the Independence Number of Random Graph Built with Markov Chain

Motivated by network models, we consider random graphs whose existence of edges is determined by a Markov process. In particular, for every $i < t$ we have a Bernoulli variable X_i^t for the edge (i,t) whose probability of success is given by $\Pr\left\{X_{i+1}^{(i)} = 1 : X_i^{(t)} = 0\right\} = \Pr\left\{X_i^{(t)} = 1\right\}$ and $\Pr\left\{X_{i+1}^{(i)} = 1 : X_i^{(t)} = 1\right\} = \delta \cdot \Pr\left\{X_i^{(t)} = 1\right\}$ where $\delta \in (0,1)$ is a decay parameter. Specifically, our model reduces to Erdös-Rényi graph if $\delta = 1$. We show that the maximum size of an independent set is $(1 + \frac{2}{3e} - e^{-h}) \cdot n$ and the size of the greedily maximal independent set is $\Omega\left(n^{1/(1+w)}\right)$ where $w = \lceil 1/(1-\delta) \rceil$. Our proof technique is to analyse a sequence of dependent Bernoulli random variables and show that for this sequence its partial sum equals to $\Theta\left(\log(n)/(1-\delta)\right)$.

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CP2
Ordering with Precedence Constraints and Budget Minimization

We introduce a variation of the scheduling with precedence constraints problem that has applications to molecular folding and production management. Given a bipartite graph $H = (B, S)$, in which vertices in B are considered as goods or services that must be bought to produce items in S that must be sold and every edge from $j \in S$ to $i \in B$ indicates the priority of i over j. The goal is to obtain an ordering of $B \cup S$ with respect to the precedence constraints and maximize the minimal net profit encountered as the vertices are processed. This optimal value is called the budget or capital investment required for the bipartite graph. We refer to our problem as the bipartite graph ordering problem.The problem is equivalent to a version of an NP-complete molecular folding problem that has been studied recently[Jn Manuch, Chris Thachuk, Ladislav Stacho, and Anne Condon. Np-completeness of the direct energybarrier problem without pseudoknots]. The present work seeks exact algorithms for solving the bipartite ordering problem. We give non-trivial polynomial time algorithms for finding the optimal solutions for bipartite permutation graphs, trivially perfect bipartite graphs, co-bipartite graphs. The ultimate goal is to completely characterize the classes of graphs for which the problem can be solved exactly in polynomial time.

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CP2
Submodular Maximization over Easy Knapsack Constraints

We consider the problem of maximizing a submodular function over multiple easy knapsack constraints. An easy knapsack is a single linear inequality, either $\leq$ or $\geq$, over binary variables such that the coefficients of this inequality form a super increasing sequence. There is also an alternative characterization with the clutter of minimal covers of this knapsack. The question we consider is interesting not only because it adds to the rich literature on approximating submodular maximization over special independence families, but also because it can be shown that any independence family can be written as the intersection of finitely many easy $\leq$ knapsacks (albeit exponentially many in general). We give several complexity results for our problem. In particular, we show that the problem can be solved in polynomial time when the number of knapsack constraints is bounded by a constant, and we show that when this number is taken as an input, there do not exist randomized polynomial time algorithms that approximate within factor $\Omega(\sqrt{n})$ where n is the dimension of each knapsack. The hardness of approximation is achieved by a PTAS reduction from a fairly general class of cardinality optimization problems.

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CP2

Attracting, Retaining, and Ensuring the Success of All Learners

Attracting, retaining and promoting the success of all learners in post-secondary education, including women, people of colour, and other marginalized groups, is an important goal and can be assisted by adapting a variety of teaching strategies. However, it is time-consuming to stay on top of the latest and most relevant research on teaching and learning mathematics. In this session, we will present a high-level overview along with strategies you can implement immediately in your classrooms and when supervising students. We will discuss critical features of inclusive math education, including contextualizing content, open-ended inquiry, role models, and the social construction of mathematics. Instructional strategies included will focus on both online and classroom instruction with actionable ideas for faculty, staff, teaching assistants, and students themselves. Strategies and materials will be demonstrated and an extensive resource list will be provided. Examples are drawn from a typical third-year discrete mathematics course.

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CP2

A Dichotomy for Approximation of H-Coloring

We study the approximability of minimum cost homomorphism (MinHOM) problem within a constant factor. Given two (di)graphs G, H and a cost function $c : (V(G), V(H)) \rightarrow \mathbb{R} \cup \{+\infty\}$, in the MinHOM($H$) problem we are interested in finding a homomorphism (a.k.a H-*coloring*) $f : V(G) \rightarrow V(H)$ that minimizes $\sum_{v \in V(G)} c(v, f(v))$. When all the costs are either zero or infinity then the MinHOM(H) becomes the list homomorphism problem LHOM(H) in which the goal is to find a homomorphism from G to H with total cost zero. When digraph H contains *digraph asteroidal triple (DAT)* then LHOM(H) becomes NP-complete, and otherwise polynomial-time solvable. It is not difficult to see when the digraph LHOM(H) is NP-complete then MinHOM(H) is not approximable. On the other hand, when H is DAT-free, we design a constant approximation algorithm for MinHOM(H). Therefore, we obtain a dichotomy classification for approximability of minimum cost homomorphism to digraphs. This somewhat comes as a surprise that the class of DAT-free digraphs draws dichotomy for both list homomorphism problem and approximation of Minimum cost homomorphism.

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CP3

Rainbow Turan Numbers

How many edges can a graph with n vertices have while still avoiding certain subgraphs? Defined in the 1940's, the Turan number of a graph H is the largest number of edges among all n vertex graphs with no H subgraph. In 2007, Keevash, Mubayi, Sudakov and Verstraete defined the rainbow Turan number of a graph H as the largest number of edges for an n vertex graph, G, such that some proper coloring of G does not contain a rainbow H subgraph. I will give a brief introduction to extremal graph theory, Turan numbers and rainbow Turan numbers before discussing results for the rainbow Turan numbers of double stars. I will also introduce generalizations of the rainbow Turan number as well as some related open problems.

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CP3

A Metric on Directed Graphs and Markov Chains Based on Hitting Probabilities

The shortest-path, commute time, and diffusion distances on undirected graphs have been widely employed in applications such as dimensionality reduction, link prediction, and trip planning. Increasingly, there is interest in using asymmetric structure of data derived from Markov chains and directed graphs, but few metrics are specifically adapted to this task. We introduce a metric on the state space of any ergodic, finite-state, time-homogeneous Markov chain and, in particular, on any Markov chain derived from a directed graph. Our construction is based on hitting probabilities, with nearness in the metric space related to the transfer of random walkers from one node to another at stationarity. Notably, our metric is insensitive to shortest and average walk distances, thus giving new information compared to existing metrics.We use possible degeneracies in the metric to develop an interesting structural theory of directed graphs and explore a related quotienting procedure. Our metric can be computed in $O(n^3)$ time, where n is the number of states, and in examples we scale up to $n = 10,000$ nodes and $\approx 38M$ edges on a desktop computer. In several examples, we explore the nature of the metric, compare it to alternative methods, and demonstrate its utility for weak recovery of community structure in dense graphs, visualization, structure recovering, dynamics exploration, and multiscale cluster detection.

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CP3

Coloring of Graphs Avoiding Bicolored Paths of a Fixed Length

The problem of finding the minimum number of colors to color a graph properly without containing any bicolored copy of a fixed family of subgraphs has been widely studied. Most well-known examples are star coloring and acyclic coloring of graphs (Grnbaum, 1973) where bicolored copies of P_4 and cycles are not allowed, respectively. In this talk, we introduce a variation of these problems and study proper coloring of graphs not containing a bicolored path of a fixed length and provide general bounds for all graphs. A P_k-coloring of an undirected graph G is a proper vertex coloring of G such that there is no bicolored copy of P_k in G, and the minimum number of colors needed for a P_k-coloring of G is called the P_k-*chromatic number* of G, denoted by $s_k(G)$. We provide bounds on $s_k(G)$ for all graphs, in particular, proving that for any graph G with maximum degree $d \geq 2$, and $k \geq 4$, $s_k(G) = O(d^{\frac{k-1}{k-2}})$. Moreover, we find the exact values for the P_k-chromatic number of the products of some cycles and paths for $k = 5, 6$.

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CP3

Flexible List Colorings in Graphs with Special Degeneracy Conditions

For a given $\varepsilon > 0$, we say that a graph G is ε-flexibly k-choosable if the following holds: for any assignment L of color lists of size k on $V(G)$, if a preferred color from a list is requested at any set R of vertices, then at least $\varepsilon|R|$ of these requests are satisfied by some L-coloring. We consider the question of flexible choosability in several graph classes with certain degeneracy conditions. We characterize the graphs of maximum degree Δ that are ε-flexibly Δ-choosable for some $\varepsilon = \varepsilon(\Delta) > 0$, which answers a question of Dvork, Norin, and Postle [List coloring with requests, JGT 2019]. In particular, we show that for any $\Delta \geq 3$, any graph of maximum degree Δ that is not isomorphic to $K_{\Delta+1}$ is $\frac{1}{6\Delta}$-flexibly Δ-choosable. Our fraction of $\frac{1}{6\Delta}$ is within a constant factor of being the best possible. We also show that graphs of treewidth 2 are $\frac{1}{3}$-flexibly 3-choosable, answering a question of Choi et al. [Flexibility of Planar Graphs – Sharpening the Tools to Get Lists of Size Four, arXiv 2020] about outer-planar graphs.

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CP4

Kissing Number in Non-Euclidean Spaces

We provide upper and lower bounds on the kissing number of congruent radius $r > 0$ spheres in hyperbolic $\mathbb{H}^n$ and spherical $\mathbb{S}^n$ spaces, for $n \geq 2$. For that purpose, the kissing number is replaced by the kissing function $\kappa_H(n, r)$, resp. $\kappa_S(n, r)$, which depends on the dimension n and the radius r. After we obtain some theoretical upper and lower bounds for $\kappa_H(n, r)$, we study their asymptotic behaviour and show, in particular, that $\kappa_H(n, r)\ const d_{n-1} e^{(n-1)r}$, where d_n is the sphere packing density in $\mathbb{R}^n$. Then we produce numeric upper bounds by solving a suitable semidefinite program, as well as lower bounds coming from concrete spherical codes. A similar approach allows us to locate the values of $\kappa_S(n, r)$ over subintervals in $[0, \pi]$ with relatively high accuracy.

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CP4

Limited Broadcast Domination in Graph Classes

A k-limited dominating broadcast on a graph G is a function $f : V \to \{0, 1, \ldots, k\}$ such that, for every vertex x with $f(x) = 0$, there exists a vertex y such that $f(y) > 0$ and $d(x, y) \leq f(y)$. The k-limited broadcast domination number of G is the minimum possible value of $\sum_{x \in V} f(x)$, where f is a a k-limited dominating broadcast on G. We describe polynomial-time algorithms for computing the k-limited broadcast domination number in graph classes including strongly chordal graphs, interval graphs and proper interval bigraphs.

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CP4

Random Embeddings: Expected Number of Faces of Complete Graph

A random embedding of a graph is given by choosing randomly and independently a local rotation of edges incident with each of the vertices. We can then study properties of the resulting embedding, in particular the number of faces (equivalently, the genus of the embedding). Random embeddings appear of sufficient interest not only in topological graph theory but also within several areas of pure mathematics and theoretical physics. The area was started by Stahl and Gross in the 80's. Stahl proved that the expected number of faces of a random embedding of a complete graph K_n is at most $n + \ln n$. We improve his bound to $3.5 \ln n + C$ and also give a lower bound of the same asymptotic order. Joint work with Jesse Campion Loth, Kevin Halasz, Tom Masark and Bojan Mohar.

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CP5

Unigraphs and Hereditary Graph Classes

A unigraph is a graph that is the unique realization of its degree sequence up to isomorphism. Most graphs are not unigraphs, but the class of unigraphs includes several remarkable families of graphs, such as the threshold graphs, the matroidal graphs, and the matrogenic graphs. Though each of these subclasses is hereditary, the class of unigraphs itself is not hereditary, though it "almost" is. We characterize the largest hereditary subclass and the minimal hereditary superclass of the unigraphs. We will see that like the classes of threshold, matroidal, and matrogenic graphs, these larger hereditary classes have several alternate characterizations in terms of forbidden subgraphs, structural decompositions, and degree sequence conditions.

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CP5

Expressing Graphs As Symmetric Differences of Cliques in the Complete Graph

Any finite simple graph G can be represented by a collection C of subsets its vertex set so that two vertices appear in an odd number of sets in C if and only if they are connected by an edge in G. The minimum cardinality of such a collection is called the clique-build number of G, denoted $\mathrm{c}_2(G)$. Such a collection induces a vector representation of G over the field of order 2, known as a faithful orthogonal representation. We explore the close relationship between $\mathrm{c}_2(G)$, the minimum dimension of a faithful orthogonal representation of G over $\mathbb{F}_2$, and the minimum rank of G over $\mathbb{F}_2$. In particular, we show that $\mathrm{mr}(G, \mathbb{F}_2) \leq \mathrm{c}_2(G) \leq \mathrm{mr}(G, \mathbb{F}_2)+1$. In the case that G is a forest, we show equality of the clique-build number and the minimum rank of G. We provide upper bounds for $\mathrm{c}_2(G)$ in terms of the number of vertices, the number of edges, and the minimum size of a vertex cover of G. Finally, we show that the graph property $\mathrm{c}_2(G) \leq k$ is hereditary and finitely defined. We exhibit the sets of minimal forbidden induced subgraphs for $k = 1$ and $k = 2$.

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CP5

KnigEgervry and Egervry Graphs

Fifty-six years ago, Jack Edmonds published his elegant characterization of the perfect matching polytope $\mathcal{P}$ of a graph $G = (V, E)$, i.e., the convex hull of the characteristic vectors of the perfect matchings of G. Edmonds described $\mathcal{P}$ polyhedrally as the set of nonnegative vectors in $\mathbb{R}^E$ satisfying two families of constraints: 'saturation' and 'blossom'. We now call graphs for which the blossom constraints are essential *Edmonds* graphs and those for which the blossom constraints are implied by the others *Egervry* graphs (aka 'BvN graphs'). As it turns out, the second graph class interacts interestingly with more familiar classes. For example, bipartite graphs are Egervry—an assertion equivalent to the Birkhoff-von Neumann Theorem on doubly-stochastic matrices. More generally, KnigEgervry graphs are Egervry. This talk introduces these ideas and shares a few results on Egervry graphs. (Joint work with Jack Edmonds and Craig Larson.)

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CP6

Efficient K-Domination in Hamming Graphs

Rubalcaba and Slater (Robert R. Rubalcaba and Peter J. Slater. Efficient (j, k)-domination. *Discuss. Math. Graph Theory*, 27(3): 409423, 2007.) define a (j, k)-*dominating function* on X as a function $f : V(X) \to \{0, \ldots, j\}$ so that for each $v \in V(X)$, $f(N[v]) \geq k$, where $N[v]$ is the closed neighbourhood of v. Such a function is *efficient* if all of the vertex inequalities are met with equality. They give a simple necessary condition for efficient domination, namely: if X is a d-regular graph on n vertices that has an efficient $(1, k)$-dominating function, then the size of the corresponding dominating set divides $n \cdot k$. The Hamming graph $H(q, d)$ is the graph on the vectors $\mathbb{Z}_q^d$ where two vectors are adjacent if and only if they are at Hamming distance 1. We show that if q is a prime power, then the previous necessary condition is sufficient for $H(q, d)$ to have an efficient $(1, k)$-dominating function. This result extends a result of Lee (Jaeun Lee. Independent perfect domination sets in Cayley graphs. *J. Graph Theory*, 37(4): 213219, 2001.) on independent perfect domination in hypercubes. We mention difficulties that arise for $H(q, d)$ when q is not a prime power.

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CP6

B-Edge Consecutive Edge Magic Total Labeling of Trees

Let $G(V, E)$ be a simple, connected, and undirected graph, where V and E are the set of vertices and the set of edges of G. An edge magic total labeling on G is a bijection $f : V \cup E \longrightarrow \{1, 2, , |V| + |E|\}$, provided that for every $uv \in$

$E, w(uv) = f(u)+f(v)+f(uv) = K$ for a constant number K. Such a labeling is said to be a super edge magic total labeling if $f(V) = \{1, 2, , |V|\}$ and a b-edge consecutive edge magic total labeling if $f(E) = \{b+1, b+2, , b+|E|\}$ with $b \geq 1$. In this research, we give sufficient conditions for a graph G having a super edge magic total labeling to have a b-edge consecutive edge magic total labeling. We also give several classes of connected graphs which have both labelings.

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CP7

On the Combinatorics of Placing Balls into Ordered Bins

We consider a particular configuration of the classic Balls in Bins counting problem: we count the number of ways to split n balls into nonempty, ordered bins so that the most crowded bin has exactly k balls. We establish closed forms for three of the different cases that can arise: $k > \frac{n}{2}$, $k = \frac{n}{2}$, and where $\exists\ j < k$ such that $n = 2k + j$. As an immediate result of our proofs, we find a closed form for the number of positive integer solutions to $x_1 + x_2 + \cdots + x_\ell = n$ with the attained maximum of the integers equalling k, and ℓ represents the number of bins in an arbitrary configuration. The problem is generalized to find a formula that enumerates the total number of ways without specific conditions on n, ℓ, and k, using only direct enumeration instead of generating functions. Subsequently, we prove various identities and properties associated with such sums and find lower and upper bounds on the generalized problem using the modified version of Stirling's approximation.

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CP7

2-Limited Broadcast Domination in Grids

Suppose there is a transmitter located at each vertex of a graph G. A k-limited broadcast on G is an assignment of the integers $0, 1, \ldots, k$ to the vertices of G. The integer assigned to the vertex x represents the strength of the broadcast from x, where strength 0 means the transmitter at x is not broadcasting. A broadcast of positive strength s from x is heard by all vertices at distance at most s from x. A k-limited broadcast is called dominating if every vertex assigned 0 is within distance d of a vertex whose transmitter is broadcasting with strength at least d. The k-limited broadcast domination number of G is the minimum possible value of the sum of the strengths of the broadcasts in a k-limited dominating broadcast of G. Observe that the 1-limited broadcast domination number of G equals the domination number of G. We give tight upper and lower bounds for the 2-limited broadcast domination of Cartesian products of paths, and of a path and a cycle.

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CP7

Density of C_{-4}-Critical Signed Graphs

Given a signed graphs (G, σ), let $g_{ij}(G, \sigma)$ $(ij \in \mathbb{Z}_2^2)$ denote the length of a shortest non-trivial closed walk whose parity of the number of negative edges is i and parity of the length is j. If (G, σ) is (H, π)-colorable, then $g_{ij}(G, \sigma) \geq g_{ij}(H, \pi)$ for each $ij \in \mathbb{Z}_2^2$. A signed graph (G, σ) is (H, π)-critical if $g_{ij}(G, \sigma) \geq g_{ij}(H, \pi)$, it admits no homomorphism to (H, π) but any proper subgraph of it does. By a signed indicator construction, we first show that the k-coloring problem of graphs is captured by the C_{-k}-coloring problem of signed graphs. Then we prove that, except for one particular signed graph on 7 vertices and 9 edges, any C_{-4}-critical signed graph on n vertices must have at least $\lceil \frac{4n}{3} \rceil$ edges, and that this bound or $\lceil \frac{4n}{3} \rceil + 1$ is attained for each value of $n \geq 9$. As an application to planarity, we conclude that every signed bipartite planar graph of negative girth at least 8 admits a homomorphism to C_{-4} and show that this bound is the best possible. This can be viewed as a bipartite analog of Grtzsch's theorem and fits into a larger framework of the study, namely analogs of Jaeger conjecture on circular flows and Jaeger-Zhang conjecture.

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CP7

Extendablility of k-Suitable Matchings in Cartesian Products

A graph G is *m-extendable* if $m < |V(G)|/2$ and every matching of size m extends to a perfect matching. The largest value for which a graph G with a perfect matching is m-extendable, called the *extendability* of G, has been studied at length. We discuss a relatively new approach for studying extendability in bipartite graphs that was initially proposed by Vandenbussche and West in 2009. In a bipartite graph G, a set $S \subseteq V(G)$ is *deficient* if $|N(S)| < |S|$. A matching M with vertex set U is *k-suitable* if $G - U$ has no deficient set of size less than k. Define the extremal function $f_k(G)$ to be the largest integer r such that every k-suitable matching in G with at most r edges extends to a perfect matching. We discuss known results on $f_k(G)$ when G is a hypercube, and show that analogous results hold for a much larger family of graphs, namely the d-fold Cartesian product graph of an even cycle. We also pose some related questions for future research.

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MS1

The Threshold Strong Dimension of a Graph

Let G be a graph, u, v and w be vertices in G. Then w is said to strongly resolve u and v if there is either a shortest u-w path that contains v or a shortest v-w path that contains u. A set W of vertices of G is a strong resolving set if every pair of vertices in G is strongly resolved by a vertex of W. A smallest strong resolving set is called a strong basis and its cardinality, the strong dimension. The smallest strong dimension among all graphs having G as spanning subgraph is called threshold strong dimension of G and is denoted by $\tau_s(G)$. We determine bounds on the threshold strong dimension of a graph and determine some structural properties of graphs with threshold strong dimension 2.

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MS1

An Edge Condition for Long Cycles in Balanced Tripartite Graphs

The circumference c of a graph G is the length of a longest cycle in G. In the event that $c = |G|$, we say that G is Hamiltonian. Finding sufficient conditions for a graph to be Hamiltonian or to have large circumference is a well-studied problem in graph theory. In 1972, Woodall found a minimum integer $g(n, k)$ such that every graph with $n \geq 2k + 3$ vertices and at least $g(n, k)$ edges has circumference at least $n - k$. Adamus solved an analogous problem for bipartite graphs in 2009. In this talk, we discuss a new edge bound which guarantees that a balanced tripartite graph has large circumference.

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MS1

Women In Graph Theory and Applications (WIGA)

Women have been getting PhDs in math at a rate well beyond what these numbers reflect. Although there has been a slow increase in the number of tenure-track women faculty in university mathematics departments, the percentage of full professors is very far from that same percentage of students. This theme opener will discuss and highlight the exceptional research from the NSF funded IMA research program Women in Graph Theory and Applications (2019). By promoting and showcasing the research done by researchers at all levels, it is hoped to encourage women to continue their pursuit of mathematics research. A common thought among women in mathematics is : A B- male can have a successful career. A woman needs to be A+ for the same to happen. What can we do to make this change for women at all career stages?

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MS1

Graphs, Codes, and Compressed Sensing

The Interval-passing algorithm (IPA) used in compressed sensing is an iterative process that is used to recover a k-sparse signal ¡b¿x¡/b¿ $\in \mathbb{R}^n$ from a linear measurement vector ¡b¿y¡/b¿ where ¡b¿y¡/b¿ $= H$ ¡b¿x¡/b¿. The matrix H is called the measurement matrix. Similar to the iterative decoder used in decoding low-density parity-check (LDPC) codes, the IPA may be modeled by a bipartite graph called a Tanner graph. Yakimenka and Rosnes showed that graphical substructures called termatiko sets characterize when the IPA fails; the size of the smallest termatiko set is called the termatiko distance. In this talk, we present new results on the structure of different types of termatiko sets as well as bounds on the sizes of termatiko sets that exist in the graphs corresponding to certain classes of measurement matrices. This work gives new insight to designing good graphs (and corresponding measurement matrices) for compressed sensing.

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MS2

Bounds on the Defective, Multi-fold, List Chromatic Number of Planar Graphs via Alon-Tarsi Number

Let G be a graph and d, m, k be natural numbers. A k-list assignment L is a map that assigns a k-set to each vertex of G. A d-defective, m-fold, L-coloring of G is a function ϕ that assigns to each vertex $v \in V$ an m-set $\phi(v) \subseteq L(v)$ so that the color class $V_\alpha := \{v \in V : \alpha \in \phi(v)\}$ of each color α induces a subgraph $G[V_\alpha]$ with maximum degree at most d. For a defective coloring, an edge is a flaw if its ends have the same color. Our main technical theorem is: Theorem. Let $K_2 = (\{u, u'\}, \{uu'\})$. For every planar graph $G = (V, E)$, the lexicographical product $G[K_2]$ has a matching M with no edge of the form $(v, u)(v, u')$, where $v \in V$, such that the Alon-Tarsi number of $G[K_2] - M$ is at most 9. Corollary. For every planar graph G there is a set F of edges inducing a subgraph in G with maximum degree 2 such that for every 9-list assignment L there is a 1-defective, 2-fold, L-coloring of G whose flaws are contained in F. The online version of the corollary also holds. The novelty of the corollary is that the set F of possible flaws does not depend on the list assignment L. The proof of the theorem uses the Combinatorial Nullstellensatz of Alon, and requires considerably more algebraic calculation than a similar result of Grytczuk and Zhu for 4-defective, 1-fold coloring of planar graphs.

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MS2

Strong 4-Colourings of Graphs

In this talk well discuss strong 4-colourings of graphs and prove two new cases of the Strong Colouring Conjecture. Let H be a graph with maximum degree at most 2, and let G be obtained from H by gluing in vertex-disjoint copies of K_4. Well show that if H contains at most one odd cycle of length exceeding 3, or if H contains at most 3 triangles, then G is 4-colourable.

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MS2

Implications in Rainbow Forbidden Subgraphs

An edge-colored graph G is *rainbow* if each edge receives a different color. For a connected graph H, G is *rainbow H-free* if G does not contain a rainbow subgraph which is isomorphic to H. By definition, if H' is a connected subgraph of H, every rainbow H'-free graph is rainbow H-free. On the other hand, in 2015, Bass, Magnant, Ozeki and Pyron discovered a kind of reverse implication. Let $K_{1,3}^+$ be the graph obtained from $K_{1,3}$ by subdividing one edge with a single vertex. They proved that every rainbow $K_{1,3}^+$-free complete graph edge-colored in 7 or more colors is rainbow $K_{1,3}$-free. Their result shows that even if H' is a connected proper supergraph of a connected H, it is possible that a rainbow H'-free complete graph edge-colored in sufficiently many colors is rainbow H-free. In this talk, we discuss this possibility. Let $K_{1,k}^+$ be the graph obtained from $K_{1,k}$ by subdividing one edge with a single vertex. We report that every rainbow $K_{1,k}^+$-free complete graph edge-colored in sufficiently many colors is rainbow $K_{1,k}$-free. We also report that this implication occurs only if (H, H') is $(K_{1,k}, K_{1,k}^+)$ for some k.

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MS2

Upper Bounds for $\Delta(\Sigma)$ where $-53 \leq \chi(\Sigma) \leq -8$

Vizing's Planar Graph Conjecture states that every planar graph of maximum degree at least 6 is class one. If for a surface Σ, we define $\Delta(\Sigma) = \max\{\Delta(G) : G$ is a connected class two graph of maximum degree Δ that is embedded in $\Sigma\}$, then one can claim that for a surface Σ, any connected graph of maximum degree Δ that is embedded in Σ is class one if $\Delta > \Delta(\Sigma)$. Further, Vizing's Planar Graph Conjecture also can be restated as $\Delta(S) = 5$ if S is a sphere.

In this talk, we will focus on $\Delta(\Sigma)$ and upper bounds for $\Delta(\Sigma)$ for surfaces Σ of characteristic $-53 \leq \chi(\Sigma) \leq -8$.

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MS3

Rainbow Saturation

We introduce Rainbow Saturation, a variation on the recent Rainbow Extremal numbers which have seen much attention.

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MS4

Matchings in K-Partite K-Graphs

Let H be a k-partite k-graph with parts $V_1, \ldots, V_k$ each of size n such that, for every $i \in [k]$, every $(k-1)$-set in $\prod_{j\in[k]\setminus\{i\}} V_j$ lies in at least a_i edges. Suppose further that $a_1 \geq \ldots \geq a_k$. Han, Zang and Zhao showed that for every $\epsilon > 0$ and sufficiently large n, with $a_1, a_2 \geq \epsilon n$, H contains a matching of size at least $\min\{n-1, \sum_{i\in[k]} a_i\}$, answering and generalising a question of Rödl and Ruciński. Their arguments use complex absorbing methods which fail when all of $a_2, \ldots, a_k$ are small. We consider the remaining cases and, in particular, show that when $\sum_{i=2}^{k} a_i \leq \sqrt{n/(k+1)}$, H in fact contains a matching of size at least $\min\{n, \sum_{i\in[k]} a_i\}$. Our proof takes a novel approach, making use of Aharoni and Haxell's 'Hall's theorem for hypergraphs' and rainbow matchings. Joint work with Richard Mycroft.

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MS4

Spherical Two-Distance Sets and Spectral Theory of Signed Graphs

A set of unit vectors in a Euclidean space is called a spherical two-distance set if the pairwise inner products of these vectors assume only two values a ¿ . It is known that the maximum size of a spherical two-distance grows quadratically as the dimension of the Euclidean space grows. However when the values a and are held fixed, a very intricate behavior of the maximum size emerges. Building on our recent resolution in the case of a + = 0, we make a plausible conjecture which connects this behavior with spectral theory of signed graphs in the regime ¡ 0 ¡ a, and we confirm this conjecture when a + 2 ¡ 0 or (1 - a)/(a -) is 1, v2 or v3. Joint work with Jonathan Tidor, Yuan Yao, Shengtong Zhang and Yufei Zhao.

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MS5

Product Power Throttling Number and Domination Number

The domination number of a graph G is a well-studied parameter. It is the size of the smallest set S of vertices so that each vertex is either in S or adjacent to a vertex in S. Thus, each vertex is "seen either initially or one step later. Other graph parameters allow vertices to be seen at later stages, such as zero forcing, power domination and "Cops and Robbers. The product power throttling number of a graph G is defined as the minimum product of the size of a set S and the longest time it takes for every vertex to be seen under power domination, with initial set S. The product power throttling number of a graph was defined to study product throttling for power domination. In this talk we compare and contrast the product power throttling numbers of a variety of graph families with their domination numbers.

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MS5

The Structure of Social Networks using Iterated Models

The Preferential Attachment Model (BarabsiAlbert, 1999) and the ACL Preferential Attachment Model (Aiello, Chung, Lu, 2001) for random networks, evolve over time and rely on the structure of the graph at the previous time step. Further models of complex networks include: the Iterated Local Transitivity Model (Bonato, Hadi, Horn, Pralat, Wang, 2011) and the Iterated Local Anti-Transitivity Model (Bonato, Infeld, Pokhrel, Pralat, 2017). Yet, these models do not tell the whole picture. In this talk we will explore two additional models that utilize applications of complex networks including social networks and internet traffic. We will focus on the structural properties of the networks described, and provide open problems into applications of complex networks.

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MS5

Breaking Symmetries: Distinguishing Mycielskian Graphs

Symmetry in a graph G can be measured by investigating possible automorphisms of G. One way to do this is to color the vertices of G in such a way that only the trivial automorphism can preserve the color classes. If such a coloring exists with d colors, G is said to be *d-distinguishable*. The smallest d for which G is d-distinguishable is its *distinguishing number*. In this talk we'll investigate this parameter in the setting of simple graphs achieved by applying the traditional Mycielskian and generalized Mycielskian constructions. The traditional Mycielskian construction was introduced by Mycielski in 1955 to prove that there exist triangle-free graphs with arbitrarily large chromatic number.

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MS6

On the Linear Arboricity Conjecture

A *linear forest* is a union of vertex-disjoint paths, and the *linear arboricity* of a graph G, denoted by $la(G)$, is the minimum number of linear forests needed to partition the edge set of G. Let G be a graph with maximum degree $\Delta(G)$. Clearly, $la(G) \geq \lceil \Delta(G)/2 \rceil$. On the other hand, the famous Linear Arboricity Conjecture (LAC) due to Akiyama, Exoo, and Harary from 1981 asserts that $la(G) \leq \lceil (\Delta(G)+1)/2 \rceil$. The conjecture has been verified for very special graphs such as planar graphs and graphs with maximum degree up to 6, and 8 and 10. A graph G is k-degenerate for a positive integer k if it can be reduced to a trivial graph by successive removal of vertices with degree $\leq k$. We prove that for any k-degenerate graph G, $la(G) = \lceil \Delta(G)/2 \rceil$ if $\Delta(G) \geq 2k^2 - k$. In conjunction with Lovasz's classic result on partitioning edge set of a graph into paths, we define a stronger version of linear forest partition and prove it holds for 2-degenerated graphs and a.a.s. for random graphs $G_{n,p}$ with a constant $p \in (0, 1)$.

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MS6

Factors of Edge-Chromatic Critical Graphs

In the 1960s, Vizing stated the now called critical graph conjectures: (1) every edge-chromatic critical graph has a 2-factor and (2) the independence number of an edge-chromatic critical graph is at most 1/2. We approximate these conjectures by showing that every edge-chromatic critical graph has a path factor. To be precise we show that they have a $\{K_{1,1}, K_{1,2}, C_{2n+1} \colon n \geq 1\}$-factor. Furthermore, for every edge e, there is a $\{K_{1,1}, K_{1,2}, C_n \colon n \geq 3\}$-factor F with $e \in E(F)$. We also study fractional matchings of edge-chromatic critical graphs. A graph is even if each of its components is Eulerian and different from K_1. We prove some sufficient conditions for the existence of an even factor in an edge-chromatic critical graph. Consequences of these results for Vizing's critical graph conjectures are discussed. (joint work with Antje Klopp and Isaak Wolf)

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MS6

Monochromatic Homeomorphically Irreducible Trees in Edge-Colored Graphs

A *homeomorphically irreducible tree* (or a *HIT*) is a tree with no vertices of degree 2. If a graph G contains a HIT T as a spanning subgraph, then T is called a *homeomorphically irreducible spanning tree* (or a *HIST*) of G. There are a lot of known results for the existence of a monochromatic tree (with some property) in edge colored graphs. For example, it was proved that every 2-edge-colored complete graph contains a monochromatic broom as a spanning tree, where a broom is a tree obtained from a star and a path by identifying the center of the star and one endpoint of the path. In this talk, we investigate monochromatic HITs and HISTs in edge-colored complete graphs.

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MS6

An Enhancement of the Erdos-Lovasz Tihany Conjecture for Line Graphs of Multigraphs

We will talk about an enhanced version of the Erdős-Lovász Tihany Conjecture for line graphs of multigraphs. That is, for every graph G whose chromatic number $\chi(G)$ is more than its clique number $\omega(G)$ and for nonnegative integer ℓ, any two integers $s, t \geq 3.5\ell + 2$ with $s + t = \chi(G) + 1$, there is a partition (S, T) of the vertex set $V(G)$ such that $\chi(G[S]) \geq s$ and $\chi(G[T]) \geq t + \ell$. In particular, when $\ell = 1$, we can obtain the same result just for any $s, t \geq 4$. The Erdős-Lovász Tihany conjecture is a special case when $\ell = 0$.

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MS8

Maximizing Five-Cycles in K_r-free Graphs

The Pentagon Problem of Erdős problem asks to find an n-vertex triangle-free graph that is maximizing the number of 5-cycles. The problem was solved using flag algebras by Grzesik and independently by Hatami, Hladk, Krl', Norin, and Razborov. Recently, Palmer suggested a more general problem of maximizing the number of 5-cycles in K_{k+1}-free graphs. Using flag algebras, we show that every K_{k+1}-free graph of order n contains at most

$$\frac{1}{10k^4}(k^4 - 5k^3 + 10k^2 - 10k + 4)n^5 + o(n^5)$$

copies of C_5 for any $k \geq 3$, with the Turn graph being the extremal graph for large enough n.

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MS8

On the Edit Distance Function of the Random Graph

Given a hereditary property of graphs $\mathcal{H}$ and a $p \in [0,1]$, the edit distance function $\mathrm{ed}_{\mathcal{H}}(p)$ is asymptotically the maximum proportion of edge-additions plus edge-deletions applied to a graph of edge density p sufficient to ensure that the resulting graph satisfies $\mathcal{H}$. The edit distance function is directly related to other well-studied quantities such as the speed function for $\mathcal{H}$ and the $\mathcal{H}$-chromatic number of a random graph. Let $\mathcal{H}$ be the property of forbidding an Erdős-Rényi random graph $G(n_0, p_0)$, and let φ represent the golden ratio. In this talk, we show that if $p_0 \in [1 - 1/\varphi, 1/\varphi]$, then we know the asymptotic value of the expectation of $\mathrm{ed}_{\mathcal{H}}(p)$ over the entire interval $p \in [0,1]$. Moreover, for any $p_0 \in [0,1]$, then we know the asymptotic value of the expectation of $\mathrm{ed}_{\mathcal{H}}(p)$ over the interval $p \in [1/3, 2/3]$.

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MS8

Trees and Tree-like Structures in Directed Graphs

In this talk I will present recent results regarding the embedding of spanning oriented trees and other tree-like directed graphs in dense directed graphs. In particular we prove that every tree on n vertices with bounded maximum degree is contained in every directed graph on n vertices with minimum semidegree at least $n/2 + o(n)$. Our results extend to a wide class of other sparse treelike structures, such as any orientation of a union of at most $o(n^{1/4})$ cycles.

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MS8

Edge-Maximal Graphs on Orientable and Some Non-Orientable Surfaces

We study edge-maximal, non-complete graphs on surfaces that do not triangulate the surface. We prove that there is no such graph on the projective plane, $K_7 - e$ is the unique such graph on the Klein bottle and $K_8 - E(C_5)$ is the unique such graph on the torus. In contrast to this for each $g > 1$, we construct an infi nite family of such graphs on the orientable surface of genus g, that are at least $(g-1)/2$ edges short of a triangulation.

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MS9

Label Propagation, Graph Convolutions, and Combinations

Semi-supervised machine learning on graphs is a widely applicable problem in network science and machine learning. Two standard algorithms, label propagation and graph neural networks, both operate by repeatedly passing information along edges, the former by passing labels and the latter by passing node features, modulated by neural networks. These two classes of algorithms have largely developed separately, and there is little understanding about the structure of network data that would make one of these approaches work particularly well compared to the other or when the approaches can be meaningfully combined. Here, we develop a random model for node attributes, based on correlations of attributes on and between vertices, that motivates and unifies these algorithmic approaches. In particular, we show that label propagation, a linearized graph convolutional network, and their combination can all be derived as conditional expectations under our model, when conditioning on different attributes.

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MS9

Reconstruction of Line-Embeddings of Stochastic Networks

Consider a random graph process with n vertices corresponding to points embedded randomly in the interval [0,1], and where edges are inserted between vertices independently with probability given by the graphon $w : [0,1]^2 -> [0,1]$. We call a graphon w diagonally increasing if, for each x, w(x,y) decreases as y moves away from x. We call a permutation σ a correct ordering if the values of the points represented by the vertices in that order, form a monotone sequence. We then ask: how can we accurately estimate σ from an observed graph? We present a randomized algorithm for finding an approximation of the correct order which, for a large class of graphons, achieves error $O^*(\sqrt{n})$ with high probability; we also show that this is the best-possible convergence rate for a large class of algorithms and proof strategies. Under an additional assumption that is satisfied by some popular graphon models, we break this "barrier" at $\sqrt{n}$ and obtain the vastly better rate $O^*(n^\epsilon)$ for any $\epsilon > 0$. These improved seriation bounds can be combined with previous work to give more efficient and accurate algorithms for related tasks, including estimating diagonally increasing graphons and testing whether a graphon is diagonally increasing.

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MS9

Network Classification and Applications to Climate Forecasting

Network models of complex systems are common in science and engineering, where nodes represent system elements, and edges represent relationships. Recently, network science-based models have found applications in analyzing climate and weather data on various spatial and temporal scales, providing new insights into several local and global climate and weather phenomena. One of the primary advantages of using networks for climate data analysis is that they provide cheap computational algorithms in several situations, where one may have to employ large scale, computational fluid dynamics models. Although climate network analysis has shown much potential, we still do not have algorithms that can be used for reliable forecasts of various climate and weather phenomena. In this talk, we will present hybrid methods that combine extra tree regression with network analysis to predict two of the most critical climate phenomena: the summer monsoon over south Asia and El NioSouthern Oscillation (ENSO). Furthermore, we will show that our method can be used for graph classification.

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MS9

Geometric Learning of Molecular Conformational Dynamics

Molecular graphs, generated from a molecule's structural formula, are a natural choice to describe molecules in AI systems, and graph neural networks (GNNs) have proven useful for the prediction of molecular properties at greatly reduced computational cost. However, the traditional definition of molecular graphs reduces the structure to 2D space and ignores information about the 3D orientation of each atom relative to the rest of the system. This omission prevents the prediction of conformational dynamics. In this work, we redefine the molecular graph to include edges between atoms within a predefined Euclidian distance to capture each atom's conformational geometry within the graph structure. With this new definition, we apply a dynamic GNN to predict changes in the relative atomic neighborhoods and atom-to-atom distances in molecular graphs of isomers of $C_7O_2H_{10}$.

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MS10

Variations of Chromatic Index

For any graph G and any class $\mathcal{F}$ of graphs, let $\chi'_{\mathcal{F}}(G) = \min\{k : G \text{ is the union of } k \text{ graphs of } \mathcal{F}\}$. If $\mathcal{F}$ consists of all matchings then $\chi'_{\mathcal{F}}$ is exactly chromatic index. In this talk the speaker will report his attempts to obtain Vizing-like theorems for a few choices of $\mathcal{F}$.

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MS10

Orientable Cycle Double Covers of Toroidal Graphs

An *orientable cycle double cover* of a graph is a collection of cycles that may be oriented to cover each edge exactly once in each direction. The Orientable Cycle Double Cover Conjecture says that every 2-edge-connected graph has an orientable cycle double cover. We verify this conjecture for graphs embeddable in the torus. The proof uses embeddings of cubic graphs: we show that every 2-connected toroidal cubic graph has a closed 2-cell embedding (in which each face is homeomorphic to an open disk and is bounded by a cycle in the graph) in some orientable surface. This last result also follows from the result of Robertson, Seymour and Thomas proving Tutte's conjecture that every 2-connected cubic graph not containing a subdivision of the Petersen graph is 3-edge-colorable. Their proof of Tutte's conjecture uses machinery similar to the proof of the Four Color Theorem. Our proof is much simpler and uses ideas that may extend to other surfaces besides the torus.

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MS10

Flows of 3-Edge Colorable Cubic Signed Graphs

Bouchet conjectured in 1983 that every flow-admissible signed graph admits a nowhere-zero 6-flow which is equivalent to the restriction to cubic signed graphs. In this paper, we proved that every flow-admissible, 3-edge colorable cubic signed graph admits a nowhere-zero 10-flow. This together with the 4-color theorem implies that every flow-admissible bridgeless planar signed graph admits a nowhere-zero 10-flow. As a byproduct, we also show that every flow-admissible hamiltonian signed graph admits a nowhere-zero 8-flow.

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MS10

Maximal k-Edge-Colorable Subgraphs, Vizing's Theorem,and Tuza's Conjecture

An easy observation about matchings in graphs is that, for any maximal matching M in a simple graph G, the vertices not saturated by M form an independent set. Such a matching can be viewed as a maximal 1-edge-colorable subgraph of G, and it is then natural to ask: what can be said about the vertices of degree less than k in a maximal k-edge-colorable subgraph of G? We prove that such vertices induce (within in the full graph G) a subgraph of maximum degree at most $k-1$, generalizing the $k=1$ observation. A stronger, more technical version of this result – which we will discuss in the talk – implies Vizing's Theorem as well as a special case of Tuza's Conjecture on packing and covering triangles.

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MS11

Erdos-Szekeres Theorem for Multidimensional Arrays

The classical Erdos-Szekeres theorem dating back almost a hundred years states that any sequence of $(n-1)^2+1$ distinct real numbers contains a monotone subsequence of length n. This theorem has been generalised to higher dimensions in a variety of ways but perhaps the most natural one was proposed by Fishburn and Graham more than 25 years ago. They defined the concept of a monotone and a lex-monotone array and asked how large an array one needs in order to be able to find a monotone or a lex-monotone subarray of size $n\times\ldots\times n$. Fishburn and Graham obtained Ackerman type bounds in both cases. We significantly improve these results. Regardless of the dimension we obtain at most a triple exponential bound in n in the monotone case and a quadruple exponential one in the lex-monotone case.

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MS11

A Proof of Tomescu's Graph-Coloring Conjecture

In 1971, Tomescu conjectured that every connected graph G on n vertices with chromatic number $k\geq 4$ has at most $k!(k-1)^{n-k}$ proper k-colorings. In this talk, we prove Tomescu's conjecture and show that equality occurs if and only if G is a k-clique with trees attached to each vertex. The key ideas are statistical importance sampling and an entropy argument.

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MS11

Rainbow Subgraphs and Their Applications

A subgraph of an edge-coloured graph is called rainbow if all its edges have distinct colours. The study of rainbow subgraphs goes back to the work of Euler on Latin squares. This talk will be about finding large rainbow trees in edge-coloured complete graphs. We will also discuss applications of this area particularly to Ringel's Tree Packing Conjecture.

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MS11

A New Nibble for Rainbow Problems

Ryser's conjecture on Latin squares made in 60s says that every Latin square of order $n\times n$ contains a transversal of order $n-1$. We show that every such Latin square contains a transversal of order $n-O(\log n)$ thus improving the previously known bound of $n-O(\log^2 n)$ by Hatami and Shor. We do so by exploiting the robust expansion properties of coloured pseudorandom graphs. This method turns out to be powerful enough for other applications as well. We obtain a new lower bound on Brouwer's conjecture on the maximum matching in Steiner triple systems, showing that every such system of order n is guaranteed to have a matching of size $n/3 - O(\log n)$. We also show that $O(n \log n)$ many symbols suffice in any generalized Latin squares to guarantee a transversal, improving on previously known bound of $n^{2-\varepsilon}$.

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MS12

Size-Ramsey Numbers of Tight Paths

The *s-colour size-Ramsey number* of a hypergraph H is the minimum number of edges in a hypergraph G whose every s-edge-colouring contains a monochromatic copy of H. We show that for every r, s and ℓ the s-colour size-Ramsey number of the ℓ-th power of a tight r-uniform path on n vertices is $O(n)$, answering a question of Dudek, Fleur, Mubayi, and Rdl (2017).

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MS12

Maximum Size Intersecting Families of Bounded Minimum Positive Co-Degree

Let $\mathcal{H}$ be an r-uniform hypergraph. The *minimum positive co-degree* of $\mathcal{H}$, denoted by $\delta^+_{r-1}(\mathcal{H})$, is the minimum k such that if S is an $(r-1)$-set contained in a hyperedge of $\mathcal{H}$, then S is contained in at least k hyperedges of $\mathcal{H}$. For $r \geq k$ fixed and n sufficiently large, we determine the maximum possible size of an intersecting r-uniform n-vertex hypergraph with minimum positive co-degree $\delta^+_{r-1}(\mathcal{H}) \geq k$ and characterize the unique hypergraph attaining this maximum. This generalizes the Erdős-Ko-Rado theorem which corresponds to the case $k = 1$. Our proof is based on the delta-system method.

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MS12

Tropicalization of Graph Profiles

A *graph profile* records all possible densities of a fixed finite set of graphs. Profiles can be extremely complicated; for instance the full profile of any triple of connected graphs is not known. To simplify these objects, we introduce their *tropicalization*. We prove that the tropicalization of a graph profile is a closed convex cone, which still captures interesting combinatorial information. We explicitly compute these tropicalizations for some sets of graphs, and relate the results to some questions in extremal graph theory.

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MS13

Efficient Generation of Clustered Hypergraphs

Hypergraphs are an increasingly popular tool for modeling network/graph data. The real networks we want to simulate are often large to begin with, and furthermore the number of possible hyper-edges becomes computationally problematic when allowing for combinations of 3 or more edges. In this work we highlight the challenges and options in efficient graph model generation to hyper-graphs. In particular we will consider generative models for clustered hypergraphs.

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MS13

Mixing Time of Stochastic Models for Chemical Reaction Networks

Chemical reaction processes and cellular processes are often modeled by reaction networks that describe the interactions between the constituent molecules. The evolution of the number of molecules are then described by a dynamical system. Such dynamical systems can be deterministic or stochastic, and they are usually challenging to analyse due to the complexity of the underlying reaction network. In this talk, I will present recent results about mixing time of Markov models associated with reaction networks, explain how stochastic analysis can help clarify the subtle discrepancies among different modeling approaches, and discuss about the insights into the dynamical or stationary behavior of the system offered by these analysis.

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MS13

Ideal Reservoir Networks for Replicating Chaos

Reservoir computers are a machine learning model that, unlike most standard models, make use of an internal complex network. Often these networks are chosen to have a real-world like topology, e.g. Barabasi-Albert, Watts-Strogatz, Erdos-Renyi, etc. To understand the effect of this network structure we trained a large number of reservoir computers to replicate the chaotic dynamics of the Lorenz attractor. Over a wide range of network topologies we found that sparse or "thinned" networks are better suited to learn the dynamics of the Lorenz attractor. To help interpret these findings we analyzed how the stability of the reservior's fixed points vary in response to the training signal. Here we found that high spectral radius and high connectivity of the network reduce the sensitivity of reservoir computers to input data, making them poorly suited for learning. This analysis offers some insight into better design principles for reservoir computers and a better understanding of the role of network topology in machine learning.

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MS13

Map Inference from Separation Times

In this talk we will discuss the use of graph layout methods to infer a geometry with limited noisy transit times between points. We apply a force-spring layout on graphs whose edges are weighted by these noisy separation times. Specifically, we explore the graph structure of US airports through open-source flight times to compare our results with the ground truth airport locations. The goal of this work is to use time series data to recover the full geometry of the data space and to find out when there is too much noise in the data or not enough data to recover an accurate geometry.

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MS14

Graph Pebbling Problems and Conjectures

Along with Min-Cost Transportation, Max Flow, Cops & Robbers, Chip Firing, and other games on graphs, Graph Pebbling fits under the umbrella of moving objects along the edges of a graph according to some rule, to achieve an objective in an optimum way. In this case, we require two pebbles to traverse an edge, one of which is consumed during traversal. The traditional paradigm seeks to minimize the number of pebbles for which any initial configuration of them on the vertices of the graph can reach any specified target vertex. In 1989 Chung used graph pebbling to solve a combinatorial number theory problem of Kleitman and Lemke; an application to abelian groups followed, as did another to p-adic Diophantine equations. Grahams conjecture on the behavior of pebbling in cartesian products has been verified in many instances but remains widely open. Generalizations to multiple targets and weighted versions soon followed, as did variations on the pebbling move (e.g. rubbling) and the objective (e.g. optimal pebbling, threshold pebbling — cops & robbers pebbling is one of the newest). Linear and integer optimization have come to bear, and complexity questions continue to be explored. A growing body of important results and techniques is emerging. This talk will be a gentle introduction to the subject, and will include a nod to the other talks in this section, with special mention of interesting conjectures and open problems that may attract newcomers.

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MS14

Stacking Results in Cover Rubbling

Let w be a positive weight function on the vertices of a graph G. If w is strictly positive, then Sjstrand and Vuong, Wyckoff independently proved a stacking theorem for w-cover pebbling, i.e., that one need only consider simple pebble distributions on G in order to determine the w-cover pebbling number of G. In this talk we consider a variant of cover pebbling, known as cover rubbling. We first use the result of Sjstrand and Vuong-Wyckoff to show that the w-cover pebbling number is equal to the w-cover rubbling number when w is strictly positive. Second, we present a stacking theorem for w-cover rubbling on trees, where w need only be supported on a dominating set.

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MS14

Pebbling in Directed Graphs

Previous work in graph pebbling has related the pebbling $\pi(G)$ to the diameter of G. Clarke, Hochberg, and Hurlbert demonstrated that every connected undirected graph on n vertices with diameter 2 has $\pi(G) = n$ unless it belongs to an exceptional family of graphs, consisting of those that can be constructed in a specific manner; in which case $\pi(G) = n + 1$. By generalizing a result of Chan and Godbole, Postle showed that for a graph with diameter d, $\pi(G) \leq n2^{\lceil \frac{d}{2} \rceil}(1 + o_n(1))$. In this talk, we continue this study relating pebbling and diameter with a focus on directed graphs. This leads to some surprising results. First, we show that in an oriented directed graph G (in the sense that if $i \to j$ then we cannot have $j \to i$), it is indeed the case that if G has diameter 2, $\pi(G) = n$ or $n + 1$, and if $\pi(G) = n + 1$, the directed graph has a very particular structure. In the case of general directed graphs (that is, if $i \to j$, we may or may not have an arc $j \to i$) with diameter 2, we show that $\pi(G)$ can be as large as $\frac{3}{2}n + 1$, and further, this bound is sharp. More generally, we show that for general directed graphs, $\pi(G) \leq 2^d n/d + f(d)$ where $f(d)$ is some function of only d.

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MS14

Stackelberg Games for Graph Pebbling and Graph Rubbling

We characterize graph pebbling and rubbling as two player Stackelberg games via bilevel integer programming. As a result, we develop novel models for the rooted graph pebbling number, the rooted 2-pebbling property decision problem, the rooted graph rubbling number and the rooted optimal rubbling number. We will describe some preliminary results implementing a computational framework for these models.

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MS15

Large Monochromatic Components

We survey some recent results regarding the size of a largest monochromatic component in an arbitrary edge coloring of a given family of (hyper)graphs. In particular, we will discuss the setting of complete (hyper)graphs, graphs with large minimum degree, random (hyper)graphs, infinite complete graphs, and Steiner triple systems.

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MS15

Rainbow Turn Number of Even Cycles

The rainbow Turn number $\mathrm{ex}^*(n, H)$ of a graph H is the maximum possible number of edges in a properly edge-coloured n-vertex graph with no rainbow subgraph isomorphic to H. We prove that for any integer $k \geq 2$, $\mathrm{ex}^*(n, C_{2k}) = O(n^{1+1/k})$. This is tight and establishes a conjecture of Keevash, Mubayi, Sudakov and Verstraete. We use the same method to prove several other conjectures in various topics. For example, we give an upper bound for the Turn number of the blow-ups of even cycles, which can be used to disprove a conjecture of Erdos and Simonovits.

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MS15

Rainbow Matchings in Hypergraphs and Tensor Rank

Given positive integers r and t, let $f(r,t)$ denote the largest f such that the following holds. There exists an r-uniform multi-hypergraph $\mathcal{H}$ and a coloring of the edges of $\mathcal{H}$ with f colors such that each colorclass is a matching of size t, but $\mathcal{H}$ contains no rainbow matching of size t. Addressing a question of Aharoni and Berger, we prove that

$$f(r,t) \leq (t-1)\binom{rt}{r},$$

which improves earlier results of Glebov, Sudakov, and Szab. Our proof is based on a result about the flattening rank of tensors.

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MS16

Greedy Matchings and Independent Sets in Random Regular Hypergraphs

We analyze two random greedy processes on sparse random graphs and hypergraphs with fixed degree sequence. We analyze the matching process, which builds a set of disjoint edges one edge at a time, and then we analyze the independent process which builds an independent set of vertices one vertex at a time. Our work generalizes and extends that of Frieze, Wormald, Brightwell, Janson and Luczak who analyzed certain instances of these processes.

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MS16

Longest Cycles in a Preferential Attachment Random Graph Model

In preferential attachment graph models, a graph is built vertex by vertex and when each new vertex arrives, it sends m new edges to older vertices, randomly, with vertices of high degree being more likely to be selected as a neighbour. One such example is the Buckley–Osthus random graph model which is a generalisation of the Barabsi–Albert preferential attachment graph model. I will discuss new bounds on the size of the longest cycles and the largest matchings in the Buckley–Osthus random graphs. These results can be used to answer a question of Frieze, Prez-Gimnez, Pralat, and Reiniger on the Hamiltonicity of the Barabsi–Albert preferential attachment graph model with parameter $m = 3$.

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MS16

Disjoint Cycles in Graphs with Restricted Independence Number

In 1963, Corrdi and Hajnal proved that every graph with at least $3k$ vertices and minimum degree at least $2k$ contains a collection of k disjoint cycles. Recently, Kierstead, Kostochka, and Yeager refined this result by describing all graphs with at least $3k$ vertices and minimum degree at least $2k-1$ that do not have k disjoint cycles. One corollary of this result is that when $k \geq 3$, every graph with $n \geq 3k$ vertices, minimum degree at least $2k-1$, and independence number at most $n-2k-1$ has k disjoint cycles. Continuing along the lines of this corollary, we will explore how relaxing the minimum degree condition affects the independence number threshold for the existence of k disjoint cycles by describing the following result. For every sufficiently small $c > 0$ and when k and n are sufficiently large $\alpha = n-2k-ck+\Theta(\sqrt{ck\log(ck)})$ is the largest number such that every graph on n vertices with independence number at most α and minimum degree at least $2k-ck$ contains k disjoint cycles.

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MS17

Excluding Immersions in Graphs with No 3-Edge-Cut

A graph G contains another graph H as an immersion if H can be obtained from a subgraph of G by repeatedly splitting off edges and deleting isolated vertices. If G contains H as an immersion, then for any integer k, the number of vertices of G with degree at least k is at least the number of vertices of H with degree at least k. We prove that the converse almost holds for graphs with no edge-cut of size 3: every H-immersion free graph with no edge-cut of size 3 can be obtained from graphs nearly violating the previous condition by using edge-sums. The condition for having no edge-cut of size 3 is necessary. One application of this result is the determination of the clustered chromatic number of H-immersion free graphs in terms of the maximum degree of H, for any fixed graph H, up to a small additive constant error.

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MS17

Clustered Coloring of Minor-Closed Graph Classes

The clustered chromatic number of a class of graphs is the minimum integer k such that for some integer c every graph in the class is k-colorable with monochromatic components of size at most c. In this talk I will discuss a conjectured characterization of minor-closed graph classes with a given clustered chromatic number, and a proof of this characterization for classes of bounded treedepth. Based on joint works with Alex Scott, Paul Seymour and David Wood.

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MS17

Obstructions for Bounded Shrub-Depth and Rank-Depth

Shrub-depth and rank-depth are dense analogues of the tree-depth of a graph. It is well known that a graph has large tree-depth if and only if it has a long path as a subgraph. We prove an analogous statement for shrub-depth and rank-depth, which was conjectured by Hlinen, Kwon, Obdrlek, and Ordyniak [Tree-depth and vertex-minors, European J. Combin. 2016]. Namely, we prove that a graph has large rank-depth if and only if it has a vertex-minor isomorphic to a long path. This implies that for every integer t, the class of graphs with no vertex-minor isomorphic to the path on t vertices has bounded shrub-depth.

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MS17

The Betti Number of the Independence Complex of Ternary Graphs

Given a graph G, the *independence complex* $I(G)$ is the simplicial complex whose faces are the independent sets of $V(G)$. Let b_i denote the i-th reduced Betti number of $I(G)$, and let $b(G)$ denote the sum of $b_i(G)$'s. A graph is ternary if it does not contain induced cycles with length divisible by three. G. Kalai and K. Meshulam conjectured that $b(G) = 2$ and $b(H) \in \{0,1\}$ for every induced subgraph H of G if and only if G is a cycle with length divisible by three. We prove this conjecture. This extends a recent results proved by Chudnovsky, Scott, Seymour and Spirkl that for any ternary graph G, the number of independent sets with even cardinality and the independent sets with odd cardinality differ by at most 1.

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MS18

Pebbling in Powers of Paths and the Strong Target Conjecture

In the way of studying the pebbling number of chordal graphs, we determined the t-pebbling number π_t of split graphs [SIAM JDM. 2014] and of semi-two-trees [DM. 2017]. In this work, we focus on another subclass of chordal graphs: power of paths. The k^{th} power $P_n^{(k)}$ of the path P_n is obtained from P_n by adding an edge between any two vertices of distance at most k from each other. In the literature there are references only for the cases $t = 1$ and $k \leq 4$. A vertex is simplicial if its neighbors form a complete graph. Chordal graphs are characterized by the existence of a simplical-vertex decomposition order. We analyze the crucial role that simplicial vertices of chordal graphs play in the unsolvable pebbling configurations. We also present our advances in the study of the following conjecture of Herscovici et al. For a target configuration $D : V(G) \to \mathbb{N}$ on a graph G, the *D-pebbling number*, $\pi(G, D)$, is defined to be the minimum number m so that from any initial configuration of m pebbles on the vertices of G, it is possible to place at least $D(v)$ pebbles on each vertex v via pebbling moves. The Target Conjecture states that $\pi(G, D) \leq \pi_{|D|}(G)$ for every target distribution D, where $|D| = \sum_v D(v)$. We introduce and provide evidence for a new Strong Target Conjecture: $\pi(G, D) \leq \pi_{|D|}(G) - (s(D) - 1)$, where $s(D)$ is the number of vertices s.t. $D(v) > 0$.

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MS18

Optimal Pebbling Number of the Square Grid

A pebbling move on a graph removes two pebbles from a vertex and adds one pebble to an adjacent vertex. A vertex is reachable from a pebble distribution if it is possible to move a pebble to that vertex using pebbling moves. The optimal pebbling number is the smallest number m needed to guarantee a pebble distribution of m pebbles from which any vertex is reachable. The optimal pebbling number of the nxm square grid graph was investigated in several papers. In this paper, we present a new method using some recent ideas to give a lower bound on the optimal pebbling number.

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MS18

On the Target Pebbling Conjecture

Graph pebbling is a network optimization model for satisfying vertex demands with vertex supplies (called pebbles), with partial loss of pebbles in transit. The pebbling number of a demand in a graph is the smallest number for which every placement of that many supply pebbles satisfies the demand. The Target Pebbling Conjecture posits that the largest pebbling number of a demand of fixed size occurs when the demand is entirely stacked on one vertex. This truth of this conjecture could be useful for attacking many open problems in graph pebbling, including the famous conjecture of Graham (1989) involving graph products. It has been proven for complete graphs, cycles, cubes, and trees. In this paper we consider 2-paths, split graphs, and Kneser graphs, important classes of graphs in graph structure theory, graph coloring, and algorithms. Using recently developed cost-related methods and induction, we prove the Target Pebbling Conjecture for all 2-paths, split graphs of minimum degree 3, and Kneser graphs with $k = 2$ and $m \geq 5$, and build tools potentially useful for attacking other graphs as well, such as, we believe, more general classes of chordal graphs.

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MS18

t-Pebbling in a Path of Complete Graphs

Given a distribution of pebbles on the vertices of a connected graph, a pebbling move removes two pebbles at a vertex and places one pebble at an adjacent vertex. One pebble is the cost of transportation. A vertex is t-reachable if at least t pebbles can be moved to the vertex using pebbling moves. The t-pebbling number of a graph is the minimum number of pebbles that ensures that any vertex is t-reachable from any initial distribution of the pebbles. A path of graphs is a path in which every vertex is replaced by a graph, and new vertices replacing old adjacent vertices are joined by edges. We determine the t-pebbling number of a path of complete graphs. This provides an example of a graph family whose t-pebbling number is the maximum of arbitrarily many linear functions in t.

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MS19

Extremal Graphs for the Tutte Polynomial

A graph transformation called the compression of a graph G is known to decrease the number of spanning trees, the all-terminal reliability, and the magnitude of the coefficients of the chromatic polynomial of a graph G. All of these graph parameters can be derived from the Tutte polynomial of G. We determine more generally compressions effect on the Tutte polynomial, recovering the previous results and obtaining similar results for a wide variety of other graph parameters derived from the Tutte polynomial. Since any simple connected graph can be transformed into a connected threshold graph via a series of compressions, this gives that threshold graphs are extremal simple graphs for all of the parameters considered.

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MS19

A Structural Result for H-Critical Graphs

Suppose G and H are simple 3-connected graphs and G has a proper H-minor. We say G is H-critical if removal of any edge either destroys 3-connectivity or the H-minor. We present a splitter-type theorem for H-critical graphs. We prove that if G is an H-critical graph and $H \neq W_3$, then one of three possibilities must occur: G/f is H-critical for some edge f; $G/f\backslash e$ is H-critical for some pair of edges e, f incident to a vertex of degree 3; or $G - w$ is H-critical for some degree 3 vertex w. Moreover, if G is H-critical, then

$$|E(G)| \leq |E(H)| + 3[|V(G|) - |V(H)|].$$

If H is the prism graph, then by Dirac's 1963 result characterizing the class of graphs with no prism minor, minimally 3-connected graphs are prism-critical graphs with two exceptions: W_{n-1} for $n \geq 4$ and $K_{3,n-3}$ for $n \geq 6$. Thus H-critical graphs may be viewed as a generalization of minimally 3-connected graphs, except that H is an arbitrary 3-connected graph and possibly highly connected. Finally, Halin proved that if G is a minimally 3-connected graph with $n \geq 8$ vertices, then $|E(G)| \leq 3n - 10$, with the exception of $K_{3,n-3}$ whose size is $3n-9$. We enhance Halin's result by identifying precisely the minimally 3-connected graphs of size $3n - 10$.

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MS19

Balanced and Unbalanced Split Graphs

A graph is a *split graph* if its vertex set can be partitioned into a clique and an independent set. A split graph is *unbalanced* if there exist two such partitions that are distinct, and *balanced* otherwise. We discuss a variety of results about balanced and unbalanced split graphs, including showing that these classes can be recognized by their degree sequences and that all threshold graphs are unbalanced split graphs.

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MS19

Complexity of C_k-Coloring in Hereditary Classes of Graphs

For a graph F, a graph G is F-free if it does not contain an induced subgraph isomorphic to F. For two graphs G and H, an H-coloring of G is a mapping $f : V(G) \to V(H)$ such that for every edge $uv \in E(G)$ it holds that $f(u)f(v) \in E(H)$. We are interested in the complexity of the problem H-coloring, which asks for the existence of an H-coloring of an input graph G. In particular, we consider H-coloring of F-free graphs, where F is a fixed graph and H is an odd cycle of length at least 5. This problem is closely related to the well known open problem of determining the complexity of 3-coloring of P_t-free graphs. We show that for every odd $k \geq 5$ the C_k-coloring problem, even in the list variant, can be solved in polynomial time in P_9-free graphs. The algorithm extends for the case of list version of C_k-coloring, where k is an even number of length at least 10. On the other hand, we prove that if some component of F is not a subgraph of a subdividecd claw, then the following problems are NP-complete in F-free graphs:

1. extension version of C_k-coloring for every odd $k \geq 5$,
2. list version of C_k-coloring for every even $k \geq 6$.

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MS20

Cycle-Free Subgraphs of Random Hypergraphs

Let $H^r_{n,p}$ denote the random r-uniform n-vertex hypergraph obtained by including each edge independently and with probability p. If $\mathcal{F}$ is a family of r-uniform hypergraphs, we let $ex(H^r_{n,p}, \mathcal{F})$ denote the size of a largest $\mathcal{F}$-free subgraph of $H^r_{n,p}$. In this talk we study this function when $\mathcal{F}$ is a family of hypergraph cycles, with a particular emphasis on the case when $\mathcal{F}$ is the set of all Berge cycles of length at most ℓ.

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MS20
Generalized Graph Saturation Problems

The generalized saturation problem asks for the minimum number of copies of H in an n-vertex F-saturated graph. This function was recently introduced by Kritschgau, Methuku, Tait, and the speaker. It has led to some interesting new results including a generalized version of the Erdos-Hajnal-Moon Theorem proved by Chakraborti and Loh in 2019. In this talk we will discuss this, and related results, with an emphasis on counting bipartite graphs in K_r-saturated graphs.

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MS21
Weighted Separators in Graphs with Sublinear Separators

Consider a graph G from a hereditary class with sublinear separators. If we assign weights to its vertices, it is not necessarily true that there exists a balanced separator of small weight (e.g., if a large fraction of the weight is placed on a universal vertex). We show this is essentially the only obstruction: For any k, a balanced separator whose weight is at most ϵ fraction of the sum of all weights exists after removal of $f_k(\epsilon) \log\log \ldots \log |V(G)|$ vertices, where the logarithm is iterated k times.

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MS21
Edge-Coloring Complex

Given a 3-colorable graph X, the 3-coloring complex $B(X)$ is the graph whose vertices are all the independent sets which occur as color classes in some 3-coloring of X. Two color classes $C, D \in V(B(X))$ are joined by an edge if C and D appear together in a 3-coloring of X. The graph $B(X)$ is 3-colorable. Graphs for which $B(B(X))$ is isomorphic to X are termed reflexive graphs. In this talk, we consider 3-edge-colorings of cubic graphs for which we allow half-edges. Then we consider the 3-coloring complexes of their line graphs. The main result is a surprising outcome that the line graph of any connected cubic triangle-free outerplanar graph is reflexive. We also exhibit some other interesting classes of reflexive line graphs.

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MS21
Packing A-Paths and Cycles with Modularity Constraints

We study the approximate packing-covering duality, known as the Erdos-Psa property, of various families of paths and cycles with modularity constraints. By refining parts of the graph minor theory to undirected group-labelled graphs, we obtain a characterization of the integer pairs L and M for which A-paths of length L mod M satisfy the Erdos-Psa property, and also some related results on cycles.

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MS21
The Extremal Function for K_{10} Minors

For positive integers t and n, the maximum number of edges that an n-vertex graph with no K_t minor can have is known as the extremal function for K_t minors. In 1968, Mader proved that for every integer $t = 1, 2, ..., 7$, a graph on $n \geq t$ vertices and at least $(t-2)n - \binom{t-1}{2} + 1$ edges has a K_t minor. Jørgensen showed that a graph on $n \geq 8$ vertices and at least $6n - 20$ edges either has a K_8 minor or is isomorphic to a graph obtained from disjoint copies of $K_{2,2,2,2,2}$ by identifying cliques of size 5. Song and Thomas further generalized the results for K_9 minors. These known extremal functions for K_t minors have been important for proving several results related to Hadwiger's conjecture for small clique minors. In this talk, I will discuss our work on the extremal function for K_{10} minors.

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MS22
More Efficient Graph Distinguishing

A coloring of a graph with colors from $\{1, 2, \ldots, d\}$ is said to be *d-distinguishing* if no nontrivial automorphism preserves the color classes. The *distinguishing number* of a graph is the smallest d for which it has a d-distinguishing coloring. One way to consider the *cost* of such a distinguishing coloring, if the original vertices are blue, is the minimum number of vertices that need to be re-colored to achieve a d-distinguishing coloring. Often, minimizing the number of colors used to distinguish G increases the cost of the distinguishing. We'll look at these definitions, and a new one, and examples, in order to find a more efficient way to distinguish a graph.

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MS22
The Distinguishing Number of Orthogonality Graphs

A graph G is said to be d *-distinguishable* if there is a labeling of the vertices with d labels so that only the trivial automorphism preserves the labels. The smallest such d is the *distinguishing number*, $\text{Dist}(G)$. A set of vertices $S \subseteq V(G)$ is a *determining set* for G if every automorphism of G is uniquely determined by its action on S. The size of a smallest determining set for G is called the *determining number*, $\text{Det}((G)$. The orthogonality graph Ω_{2k} has vertices which are bitstrings of length $2k$ with an edge between two vertices if they differ in precisely k bits. We show that $\text{Det}(\Omega_{2k}) = 2^{2k-1}$ and that if $\binom{m}{2} \geq 2k$, then $2 < \text{Dist}(\Omega_{2k}) \leq m$.

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MS22

Switchable 2-Colouring is Polynomial

A (m, n)-mixed graph is a mixed graph whose edge set is partitioned into m colours, and whose arc set is partitioned into n colours. Let G be a (m, n)-mixed graph, Γ be a permutation group acting on the colours of G, and $\pi \in \Gamma$ be a permutation. We define *switching a vertex v* with respect to π as applying π on the colour of each edge incident to v and on the colour and direction of each arc incident to v. Given an (m, n)-mixed graph G, we study of the question "Is there a sequence of switchings so that the resulting (m, n)-mixed graph admits a homomorphism to a 2-vertex target?" We show that this problem is polynomial for all Γ.

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MS22

Cycles in Color-Critical Graphs

Tuza [1992] proved that a graph with no cycles of length congruent to 1 modulo k is k-colorable. We prove that if a graph G has an edge e such that $G - e$ is k-colorable and G is not, then for $2 \leq r \leq k$, the edge e lies in at least $\prod_{i=1}^{r-1}(k-i)$ cycles of length $1 \mod r$ in G, and $G-e$ contains at least $\frac{1}{2}\prod_{i=1}^{r-1}(k-i)$ cycles of length $0 \mod r$. A (k, d)-coloring of G is a homomorphism from G to the graph $K_{k:d}$ with vertex set $\mathbb{Z}_k$ defined by making i and j adjacent if $d \leq j - i \leq k - d$. When k and d are relatively prime, define s by $sd \equiv 1 \mod k$. A result of Zhu [2002] implies that G is (k, d)-colorable when G has no cycle C with length congruent to is modulo k for any $i \in \{1, \ldots, 2d-1\}$. In fact, only d classes need be excluded: we prove that if $G - e$ is (k, d)-colorable and G is not, then e lies in at least one cycle with length congruent to $is \mod k$ for some i in $\{1, \ldots, d\}$. Furthermore, if this does not occur with $i \in \{1, \ldots, d-1\}$, then e lies in at least two cycles with length $1 \mod k$ and $G - e$ contains a cycle of length $0 \mod k$.

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MS23

Enumerative Nordhaus-Gaddum Inequalities

Nordhaus and Gaddum proved the following inequalities that give upper and lower bounds on the sum and product of the chromatic number of a graph and its complement.

$$2\sqrt{n} \leq \chi(G)+\chi(\overline{G}) \leq n+1 \quad \text{and} \quad n \leq \chi(G)\chi(\overline{G}) \leq \frac{(n+1)^2}{4}.$$

Inspired by these results, Nordhaus-Gaddum inequalities have been studied for many other graph invariants. Recently, Wagner gave a lower bound on the sum of the number of dominating sets in a graph on its complement. In this talk, we discuss some related results and their connections to well-known areas of study in graph theory.

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MS23

New Results and Open Problems in (t, R) Broadcast Domination

Domination theory is a subfield within graph theory that aims to describe subsets of the vertices of a graph which satisfy certain distance properties. The original domination problem asked one to find subsets of the vertices of a graph (with minimal cardinality) so that every vertex in the graph was either in the set or adjacent to a vertex in the set. Since its development, thousands of papers on domination theory and its many variants have appeared in the literature. We focus our study on (t, r) broadcast domination, a variant with a connection to the placement of cell-phone towers, where some vertices send out a signal to nearby vertices (with the signal decaying linearly along edges according to distance), and where all vertices must receive a minimum predetermined amount of this signal. The overall goal is to minimize the number of tower vertices needed to have all vertices receive the appropriate amount of signal reception. We summarize our past work and present a variety of open problems in this field.

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MS23

Bounding the K-Rainbow Total Domination Number

A k-rainbow dominating function of a graph G is the following: a function f which assigns a subset of $[k] = \{1, 2, \ldots, k\}$ to each vertex of G, such that if a vertex v is assigned the empty set, then the values assigned to v's neighbors union to $[k]$. A k-rainbow *total* dominating function is a function f which satisfies the following additional condition: if a vertex is assigned a singleton set $\{i\}$ then for some neighbor u, we have $i \in f(u)$. In either case, the weight of f is $\sum_{v \in V(G)} |f(v)|$. For a graph G, the k-rainbow domination number is defined as the minimum weight k-rainbow dominating function for G, and the k-rainbow *total* domination number is defined as the minimum weight k-rainbow *total* dominating function for G. We present bounds on the rainbow *total* domination number in terms of the usual domination number, the total domination number, the rainbow domination number and the rainbow total domination number. One of the main results lower bounds the rainbow total domination number in terms of the usual domination number, generalizing a result of Goddard and Henning (2018). Along with a number of partial results, we present questions and conjectures, including a Vizing-like conjecture about graph products for the rainbow total domination number.

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MS23

Strongly Regular Multigraphs

Strongly regular graphs have a direct connection to structures in algebraic combinatorics. They are defined by 4 parameters, n, k, a, and c where n is the number of nodes, k is the degree of each node, a is the number of common neighbors for every adjacent pair of nodes, and c is the number of common neighbors for every nonadjacent pair of nodes. A multigraph is a graph that has no self-loops, but may have multiple edges and is formally defined by specifying a graph G and assigning a multiplicity to each edge of G. We examine underlying strongly regular multigraphs in order to further clarify their properties, specifically with regard to combinatorial configurations. This is joint work with Leah H. Meissner.

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MS24

Maximum Number of Almost Similar Triangles in the Plane

A triangle T' is ε-similar to another triangle T if their angles pairwise differ by at most ε. Given a triangle T, $\varepsilon > 0$ and $n \in \mathbb{N}$, Brny and Fredi asked to determine the maximum number of triangles $h(n,T,\varepsilon)$ being ε-similar to T in a planar point set of size n. We show that for almost all triangles T there exists $\varepsilon = \varepsilon(T) > 0$ such that $h(n,T,\varepsilon) = n^3/24(1 + o(1))$. Exploring connections to hypergraph Turán problems, we use flag algebras and stability techniques for the proof.

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MS24

Many Cliques in Bounded-Degree Hypergraphs

In the past few years there has been substantial progress in the general area of extremal enumeration problems: determining the maximum or minimum number of substructures of a certain type in a graph or hypergraph satisfying certain conditions. In this talk I will discuss the recent resolution of some graph problems concerning cliques in graphs of bounded degree, and also discuss recent work about generalizing to hypergraphs.

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MS24

Super-Pancyclic Hypergraphs

We say a hypergraph H is super-pancyclic if for every set of vertices A, there exists a Berge cycle of H whose base vertices are exactly the vertices in A. In this talk, we give necessary conditions for a hypergraph to be super-pancyclic and also prove that these conditions are sufficient in certain classes of hypergraphs. We will also discuss related problems for finding Berge cycles in hypergraphs.

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MS24

Low Diameter Monochromatic Covers of Complete Multipartite Graphs

Define the tree cover number, $tc_r(G)$, of a graph G to be the minimum number such that for any r coloring of $E(G)$ there exists $tc_r(G)$ connected monochromatic components covering all vertices. Ryser's conjecture relates this value to the independence number of G, stating that $tc_r(G) \leq (r-1)\alpha(G)$. In this talk, we consider a strengthening of this conjecture that requires the monochromatic components to be not only connected, but also of bounded diameter. We define a function which maps a graph G to the smallest value d such that if we consider any r coloring of the edges of our graph we may find $tc_r(G)$, the tree cover number, monochromatic components, which are not necessarily trees, each of diameter at most d covering all vertices. Restricting ourselves to 2 colors, we completely classify the function for complete tripartite graphs, showing that it evaluates to 2, except for a few graphs on a small number of vertices, where it evaluates to 3. We also provide some results towards a classification of the function for complete multi-partite graphs where each part has a fixed size, but the number of parts tends towards infinity.

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MS26
Representation of Antimatroids by Convex Shapes

Antimatroid is known as a formal set system based on the anti-exchange axiom. Among many applications is the modeling the state of human knowledge, discussed in recent article by H. Yoshikawa, H. Hirai and K. Makino [Journal of Mathematical Psychology, 2016]. A typical approach to study antimatroids is to consider a closure system formed by complements of feasible sets of antimatroid. Such closure systems are known as *convex geometries*. There was a considerable progress in understanding a finite antimatroid through an associated convex geometry by representing the latter using convex shapes in Euclidean space as elements of the base set and a version of the convex closure as a closure operator. The goal of such representation was to use geometry of some low dimensional spaces. In this talk we give a survey of recent results about representations of finite antimatroids or convex geometries of small convex dimension, including results of the author with M. Bolat [Discrete Mathematics, 2019] and G. Gjonbalaj [Algebra Universalis, 2019]. Other related results were reported by G. Czdli, L.L. Stach, . Kurusa, M. Richter, L.G.Rogers and J. Kincses.

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MS26
A "Challenging Question" of Bjorner from 1976: Every Infinite Geometric Lattice of Finite Rank Has a Matching

It is proven that every geometric lattice of finite rank greater than 1 has a matching between the points and hyperplanes. This answers a question of Plya Prize-winner Anders Bjrner from the 1981 Banff Conference on Ordered Sets, which he raised as a "challenging question' in 1976.

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MS26
Designing Graph-Based Codes for Window Decoding

Low-density parity-check (LDPC) codes are a class of linear codes defined by sparse parity-check matrices and have corresponding sparse bipartite graph representations. They have been shown to be capacity-achieving over many channels using low complexity graph-based iterative decoders. Spatially-coupled LDPC (SC-LDPC) codes are a special class of codes whose repetitive graph structure makes them amenable to window decoding, in which the nodes are decoded in groups from one end to the other. This type of decoding is useful for applications such as data streaming. In this talk we show how to make the subgraph seen by the window decoder have desirable distance properties and compare these to the properties of the overall code.

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MS26
Chains in Geometric Lattices

In constructing examples, it is often useful to view lattices as join semilattices generated by ordered sets. We discuss methods of testing lattice properties, such as semidistributivity and semimodularity. In particular, we consider various versions of the Exchange Property.

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IP1

Opening Remarks and Presentation: Mixed Integer Bilevel Optimization

In bilevel optimization there are two decision makers, commonly denoted as the leader and the follower. Decisions are made in a hierarchical manner: the leader makes the first move, and then the follower reacts optimally to the leaders action. It is assumed that the leader can anticipate the decisions of the follower, hence the leader's optimization task is a nested optimization problem that takes into consideration the followers response. In this talk we focus on branch-and-cut algorithms for dealing with mixed-integer bilevel linear programs (MIBLPs). We focus on a subfamily of MIBLPs in which the leader and the follower share a set of items, and the leader can select some of the items to inhibit their usage by the follower. Interdiction Problems, Blocker Problems, and Critical Node/Edge Detection Problems are some examples of optimization problems that satisfy these conditions. We show how modeling of these problems as two-player Stackelberg games leads to integer programming formulations in the natural space of the variables. We also demonstrate how solving these problems using branch-and-cut algorithms often outperforms state-of-the-art methods from literature.

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IP2

Local Minima, Stable Sets, and Sums of Squares

We characterize the complexity of finding a local minimizer of a polynomial optimization problem as a function of the degrees of its defining polynomials. The talk will highlight the following two results: (1) Unless P=NP, there cannot be a polynomial-time algorithm that finds a point within Euclidean distance c^n (for any constant $c \geq 0$) of a local minimizer of an n-variate quadratic polynomial over a polytope. This result (even with $c = 0$) settles a question that had remained open since 1992. (2) A local minimizer of a cubic polynomial can be efficiently found by solving semidefinite programs of size linear in the number of variables. (This, as we show, stands in contrast to the fact that the seemingly easier task of finding a critical point of a cubic polynomial is strongly NP-hard.) The proofs of statements (1) and (2) revolve around the concepts of "stable sets' from graph theory and "sum of squares polynomials' from algebra. In the final part of the talk, we connect these two notions by giving an algebraic characterization of "perfect graphs' (i.e., graphs in which the size of the largest stable set of every induced subgraph equals the chromatic number of the complement of that subgraph). We show that a graph is perfect if and only if certain nonnegative polynomials associated with the graph are sums of squares. Joint work with Jeffrey Zhang (CMU) and Cemil Dibek (Princeton).

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IP3

Polynomial Optimization and Optimal Control

The moment-sum-of-squares hierarchy allows to solve globally nonconvex optimization problems with polynomial data at the price of solving a family of convex relaxations of increasing size, typically semidefinite programming problems. The propose of the talk is to explain how this approach can be extended to polynomial optimal control, what are the convergence guarantees of the hierarchy in this case, and how optimal trajectories can be approximated from the solutions of the convex relaxations.

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IP4

Kronecker-Factored BFGS and L-BFGS Methods for Deep Learning

Solving deep learning problems efficiently and effectively requires specialized optimization algorithms. Due to the enormous amounts of data used to train deep neural network (DNN) models and the huge numbers of model parameters that need to be learned by minimizing a suitable loss function, stochastic first-order methods are usually relied upon. In this talk we present, what we believe to be, the first practical quasi-Newton method for training DNNs. Because computing and storing a full BFGS or a limited-memory L-BFGS approximation is impractical, we approximate the Hessian by a block-diagonal matrix, and use the structure of the gradient and Hessian to further approximate these blocks, each of which corresponds to a layer, as the Kronecker product of two much smaller matrices, analogous to the approach in KFAC for approximating the Fisher matrix in a stochastic natural gradient method. Also, due to the indefinite and volatile nature of the Hessian with respect to changes in the parameters of a DNN, we propose a damping approach to keep the BFGS and L-BFGS approximations positive definite and to control the size of the changes in them. In tests on autoencoder feed-forward and convolutional DNN models, our methods outperformed KFAC and were competitive with state-of-the-art first-order stochastic methods.

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IP5

Weighted Linear Matroid Parity

Matching and matroid intersection are two primary frameworks of combinatorial optimization problems that admit polynomial-time algorithms. As a common generalization of these two frameworks, the matroid parity (or matroid matching) problem was introduced in the 70s. This framework is so general that it requires in the worst case an exponential number of independence oracle calls. Nevertheless, Lovsz (1980) showed that this problem admits a min-max formula and a polynomial-time algorithm for linearly represented matroids. Since then efficient algorithms have been developed for the linear matroid parity problem, which finds applications in various fields including electric circuit analysis, combinatorial rigidity theory, and topological graph theory. Recently, the weighted version of the linear matroid parity problem turned out to be solvable in polynomial time. The algorithm builds on a polynomial matrix formulation using Pfaffian and adopts a primal-dual approach based on the augmenting path algorithm of Gabow and Stallmann (1986) for the unweighted problem. In contrast to the weighted matching and matroid intersection, the algorithm does not rely on polyhedral description.

This talk provides an overview of matroid parity, putting emphasis on the weighted linear matroid parity algorithm and its applications.

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IP6

Tailored Discrete Concepts in PDE Constrained Optimization

Optimization problems with PDE constraints inherit a lot of structure introduced by the governing PDE. The talk addresses discrete concepts which are aligned to this structure while introducing as less as possible, but as much as necessary degrees of freedom on the discrete level to guarantee a prescribed quality of the approximation. The key ingredient to achieve this is the discrete treatment of the control variable. In addition, tailored numerical solution algorithms are proposed. Many ad-hoc approaches in PDE constrained optimization use fully discrete schemes which e.g. lead to *over-discretization* of the optimization problem and thus introduce unnecessary degrees of freedom for the optimization problem. This can be avoided through a sophisticated treatment of the control variable on the discrete level, whose *discrete* structure can be controlled through the discretization of the PDE and its adjoint. Our discrete concepts are applicable to the whole range of modern PDE constrained optimization, including distributed and boundary control problems, sparse optimal control problems, problems with measure controls, estimation of fully distributed parameters (control in the coefficients), and also to shape optimization. This will be illustrated by several numerical examples.

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SP1

Closing Remarks and Presentation: SIAM Activity Group on Optimization Best Paper Prize Lecture: Semidefinite Approximations of the Matrix Logarithm

The matrix logarithm, when applied to Hermitian positive definite matrices, is concave with respect to the positive semidefinite order. This operator concavity property leads to numerous concavity and convexity results for other matrix functions, many of which are of importance in quantum information theory. In this talk we show how to approximate the matrix logarithm with functions that preserve operator concavity and can be described using the feasible regions of semidefinite optimization problems of fairly small size. Such approximations allow us to use off-the-shelf semidefinite optimization solvers for convex optimization problems involving the matrix logarithm and related functions, such as the quantum relative entropy. The basic ingredients of our approach apply, beyond the matrix logarithm, to functions that are operator concave and operator monotone. As such, we introduce strategies for constructing semidefinite approximations that we expect will be useful, more generally, for studying the approximation power of functions with small semidefinite representations.

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SP2

SIAM Activity Group on Optimization Early Career Prize Lecture: Optimality in Optimization

I will discuss what it means for a method to be optimal in optimization and machine learning. When a method matches a lower bound, does that mean the method is good? How can we develop lower bounds and optimality results that are meaningful? Can theoretical results actually direct progress in what we do? While much of this talk will cover my collaborators' and my work, as well as other's results, parts will be speculative.

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JP1

Joint Plenary Speaker with the 2021 SIAM Annual Meeting (AN21): Augmented Lagrangians and Problem Decomposition in Optimization

An important approach to solving large-scale problems in optimization is decomposing them iteratively into subproblems that are easier to handle numerically. This has long been associated with exploiting block-separable structure in the primal variables by way of solving a dual problem derived from convexity. Without such convexity, problem decomposition techniques have lacked an adequate platform for development. Augmented Lagrangians in nonlinear programming have been recognized as creating local convex duality around a locally optimal solution, but in doing so they thwart decomposition by disrupting separability. Now, however, a path to problem decomposition has opened up that can utilize augmented Lagrangian methodology even in territory beyond just nonlinear programming.

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CP1

Infinite-Dimensional Generalized Nash Equilibrium Problems Arising from Energy Markets

Motivated by the current evolution of energy markets, we investigate Generalized Nash equilibrium problems where each player look to maximize their profit by exchanging goods. The time and space evolution of the goods obeys a partial differential equation, which enters the game as a shared constraint for all players. Motivated by possible economical interpretations of the solution to this game, we concentrate ourselves to the solution concept of variational equilibrium. Under appropriate regularity and convexity assumptions, such solution also satisfies a variational inequality. This enables us to study the existence of a variational equilibrium via this infinite dimensional variational inequalities. We illustrate the findings on a stylized gas market with an oligopoly setup.

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CP1

A Cooperative Game for Optimal Multiuser Power Control in Satellite Communication

Our research revolves around investigating optimal strategies in satellite communication systems to precisely allocate power among multiuser terminals who share a frequency-selective Gaussian interference channel. These terminals are competing for limited radio resources to meet their respective data rates. A discrete cooperative game model has been proposed in this study to visualize each optimal spectrum management strategy in multiuser frequency selective interference channels. The KKT conditions for this model have be analyzed and solved to get optimal solutions under symmetric conditions. This gives the optimal control scheme with regards to the direct channel gain and the noise power spectrum density.

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CP1

Stochastic Bounds in Bilevel Programming

Bilevel programming stems from the seminal work of H. von Stackelberg in the 30s, and has extensively gained in popularity in the last thirty years, as it allows to adequately model many real-life situations. More recently, stochasticity has been considered in bilevel optimization in order to model situations involving uncertainty. In classical stochastic optimization, it is common to study bounds to evaluate the efficiency and relevance of a stochastic model, where the most used ones are *the value of the stochastic solution* (VSS) and *the expected value of perfect information* (EVPI). In this presentation, we show how to adapt the classic stochastic bounds to the bilevel programming setting. Even more, we propose a new indicator, that we call *the value of shared information* (VSI), which captures the impact of a leader sharing information with the followers. We provide academic examples showing that the VSI is independent of the EVPI and the VSS, and we present an application to ridesharing companies (Uber, Lyft) where the company must decide whether to forecast the demand or not, and whether to share that information with the drivers.

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CP1

Well-Posedness of Deterministic Bilevel Games Through a General Stochastic Approach

Bilevel games, also known as Stackelberg games and Multi-Leader-Follower games, where fist introduced by H. Von Stackelberg in the 30's to model hierarchical decision problems. In the last few decades they have attracted the attention of many researchers due to their vast modeling applications and their inherent challenging structure. In this presentation, we propose a unifying approach for bilevel games, called the stochastic approach, which solves the ambiguity that arises when optimal responses of followers are not unique. This model provides a spectrum of alternatives between the classic optimistic and pessimistic approaches and includes, to the best of our knowledge, all other approaches already proposed in the literature. We model how leaders anticipate the followers' reaction as decision-dependent probability distributions, which we call beliefs. Several constructions of beliefs and results of existence of solutions are provided, particularly for bilevel games with a single follower.

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CP1

Multi-Scale Control of Stackelberg Games

We present a linear–quadratic Stackelberg game with a large number of followers and we also derive the mean field limit of infinitely many followers. The relation between optimization and mean field limit is studied and conditions for consistency are established. Finally, we propose a numerical method based on the derived models and present numerical results.

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CP1

Cooperative Game for Optimal Multiuser Power Control in Satellite Communication

Our research investigates optimal control strategies for satellite communication systems to allocate power among competing user terminals who share a multiuser frequency selective interference channel, and would be competing for limited radio resources to meet their selfish data rates. This class of optimal power resource allocation problems for a satellite transponder power subsystem is classified as a weighted sum gain optimization problem, so a discrete cooperative game model has been set up to study optimal power control strategies for transponders. The KKT condition for the game model has be analyzed and solved analytically to get optimal solutions under symmetric conditions, which gives the optimal power control scheme in terms of the channel gain and the power noise ratio.

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CP2

Distributionally Robust Expected Residual Minimization for Stochastic Variational Inequalities

The stochastic variational inequality problem (SVIP) is an equilibrium model which involves random variables and has been widely used in economics, engineering, and others. The expected residual minimization (ERM) is known as one of models to get a reasonable solution to SVIP, and its objective function is an expected value of a suitable merit function for the SVIP. However, the ERM is restricted to the case where the distribution is already known. We extend the ERM so that robust solutions can be obtained for the SVIP with uncertainty distribution (we call the extended one DR-ERM), where the worst case distribution is taken from a set which consists of probability measures whose expected value and variance take the same sample mean and variance, respectively. Under suitable assumptions, we show that the DR-ERM can be reformulated as a deterministic convex nonlinear semidefinite programming.

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CP2

Discrete-Continuous Robust Optimization Requiring Only Inexact Worst-Case Evaluations

Currently, there are few approaches available for general nonlinear robust optimization, which typically require restrictive assumptions on the adversarial problem or do not guarantee robust protection. We present an algorithm that combines outer approximation and a bundle method and which is applicable to convex mixed-integer nonlinear robust optimization problems requiring only inexact worst-case evaluations. In particular, our method does not rely on a specific structure of the adversarial problem and allows it to be nonconvex. As robust protection requires a global solution of the adversarial problem, it is a main challenge in such a general nonlinear setting. Our method requires these evaluations only up to a certain precision. For example, approximating a nonconvex adversarial problem via piecewise linearization and solving the resulting problem up to any requested error, the required assumptions are met. We model a robust optimization problem by a nonsmooth mixed-integer nonlinear problem and tackle it by an outer approximation approach that requires only inexact function values and subgradients. For the arising nonlinear subproblems, we present an adaptive bundle method. We prove its convergence to approximate critical points and, as a consequence, finite convergence of the outer approximation method. As an application, we study the gas transport problem under uncertainties on realistic instances and provide computational results showing the efficiency of the method.

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CP2

Robust Shape Optimization of An Electric Motor with Reduced Order Models

We examine the optimization of an asynchronous electrical machine. Our goal is to find the optimal width and height of conductive bars, located in the machines rotor, such that the joule losses in these bars are minimized while a given torque is preserved. The state of the machine can be described by the magnetoquasistatic approximation of Maxwell's equations coupled with circuit equations describing the windings in the stator and the bar network in the rotor. This leads to a system of partial differential algebraic equations (PDAE). On the startup of the machine, huge forces are acting on the openings of the rotor bar slots and can deform them. Therefore we treat the opening widths as uncertain and address these uncertainties with a worst-case approach. This approach leads to a bi-level structured problem which is difficult to treat numerically. We therefore employ a strategy utilizing a quadratic approximation of the robust formulation as a surrogate model combined with an adaptive strategy to control the introduced error. Since the discretization of the PDAE system leads to a system with a huge amount of degrees of freedom, we use model order reduction techniques in the form of the proper orthogonal decomposition to reduce the systems complexity. Numerical results are presented.

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CP2

Maximal Uncertainty Sets in Robust Optimization

The radius of robust feasibility (RRF) determines a value for the maximal "size" of the uncertainty set such that robust feasibility of the considered uncertain optimization problem can be guaranteed. In this talk, we focus on the RRF for mixed-integer problems (MIPs) whereas the corresponding literature focuses on continuous optimization problems. We first analyze relations between the RRF of a MIP and its continuous linear (LP) relaxation and derive conditions under which a MIP and its LP relaxation have the same RRF. In contrast to the setting commonly used in the literature, we then consider a potentially different uncertainty set for every constraint that is not necessarily full-dimensional. Thus, we extend the RRF to include "safe" variables and constraints, i.e., uncertainties do not affect certain variables or constraints. This allows for the RRF to be applied to a large variety of optimization problems and uncertainty sets. It further makes it possible to compute a "most robust" solution with respect to the size of the uncertainty set such that the costs for integrating data uncertainties stay within an a priori defined budget. We then present first methods for computing the RRF of LPs as well as of MIPs with safe variables and constraints. We finally show that the new methodologies can be successfully applied to instances in the MIPLIB for computing the RRF.

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CP2

ALSO-X and ALSO-X+: Better Convex Approximations for Chance Constrained Programs

Chance constrained programs (CCPs) are generic frameworks for decision-making under uncertain constraints. The objective of a CCP is to find the best decision that violates the uncertainty constraints within the prespecified risk level. A CCP is often nonconvex and is difficult to solve to optimality. This paper studies and generalizes the ALSO-X, originally proposed by Ahmed, Luedtke, SOng, and Xie (2017), for solving a CCP. We first show that the ALSO-X resembles a bilevel optimization, where the upper-level problem is to find the best objective function value and enforce the feasibility of a CCP for a given decision from the lower-level problem, and the lower-level problem is to minimize the expectation of constraint violations subject to the upper bound of the objective function value provided by the upper-level problem. This interpretation motivates us to prove that when uncertain constraints are convex in the decision variables, ALSO-X always outperforms the CVaR approximation. We further show (i) sufficient conditions under which ALSO-X can recover an optimal solution to a CCP; (ii) an equivalent bilinear programming formulation of a CCP, inspiring us to enhance ALSO-X with a convergent alternating minimization method (ALSO-X+); (iii) extensions of ALSO-X and ALSO-X+ to solve distributionally robust chance constrained programs (DRCCPs) under Wasserstein ambiguity set. Our numerical study demonstrates the effectiveness of the proposed methods.

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CP2

On Distributionally Robust Optimization using Integral Probability Metrics and Reproducing Kernel Hilbert Spaces

We study distributionally robust optimization (DRO) using the reproducing kernel Hilbert spaces (RKHS) and integral probability metrics (IPM), of which the type-1 Wasserstein distance is a special instance. We use RKHSs to construct a wide range of ambiguity sets, which can be viewed as generalizing finite-order moment bounds to infinite orders. This perspective unifies multiple existing robust and stochastic optimization methods. We prove the generalized variational duality for DRO, reformulating the inner moment problem into the dual program that searches for RKHS functions. Furthermore, we provide finite-sample performance guarantees of our method by leveraging convergence rate for empirical kernel mean embedding. Finally, We study the function approximation aspect of DRO, by comparing the Moreau-Yosida regularization, used in Wasserstein DRO, and kernel-based function approximation. Our analysis highlights the roles that function approximation plays in enforcing distributional robustness, especially when used with loss functions involve complex function classes.

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CP3

Automatically Extracting Differential Equations from Data with Sparse Regression Techniques

As data-centric engineering continues to expand and we proceed to collect, store, and manipulate data in more prolific quantities, the ability to automatically extract governing equations from this information remains a crucial challenge in the fields of data science and engineering. Currently, engineers construct generalized linear models manually to identify, expand, and forecast these systems over time; a process better known as system identification. With this process, the only assumption is that just a few essential terms regulate the dynamics of the model's underlying structure, which holds for many physical systems (Brunton et al., 2016). Therefore, we represent the equations using a sparse functional basis. Here, we aim to develop a method to determine equations automatically since these data sets are often otherwise intractable. We thus employ several optimization techniques to perform system identification by extracting a sparse solution for these dynamic equations to visualize and interpret the data accurately. In this work, we outline our Automatic Sparse Regression (TAPER) algorithm, which provides an iterative process that implements various statistical learning methods to extract governing equations from data. The TAPER algorithm develops a fully automated process for the identification of the Lorenz chaotic system with a precision that offers advancement to state-of-the-art semi-automated methods by at least one order of magnitude (Brunton et al., 2016).

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CP3

On a New Shape Derivative Formula for Solving a

Free Boundary Problem

In this work, we deal with numerical method for the approximation of a class of free boundary problem, which consist in minimizing an appropriate general cost. We show the existence of the shape derivative of the cost functional and express it by means of support functions, using the formulas proposed in [A. Boulkhemair, A. Chakib, On a shape derivative formula with respect to convex domains, Journal of Convex Analysis, 21 (2014), n 1, 67-87.] for a family of convex domains. Then the numerical discretization is performed using the boundary element method in order to avert the remeshing task required when one use the finite element method. Finally, we give some numerical results, based on the gradient method, showing the efficiency of the proposed approach.

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CP3

Numerical Approximation of Optimal Boundary Control Problems for Hyperbolic Conservation Laws

We discuss boundary control problems for hyperbolic conservation laws. Since solutions may develop discontinuities after finite time and/or some applications require discontinuous boundary data, a consistent numerical approximation of such problems is challenging. In this talk we focus on the numerical approximation of the adjoint gradient representation for reduced tracking-type objective functionals, which are represented by the reversible solution of a suitable adjoint equation. To this end we propose consistent numerical approximation of these optimal boundary control problems for scalar hyperbolic conservation laws, where we consider conservative finite difference schemes with corresponding sensitivity and adjoint scheme. We introduce convenient characterizations of the solutions for the adjoint equation in the case of boundary control, which are suitable to show that the limit of discrete adjoints is in fact the reversible solution of the adjoint equation. Choosing suitable approximations for the boundary controls, the convergence of discrete sensitivities to the correct solution of the sensitivity equation is obtained by a duality relation.

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CP3

Inexact Second-Order Adjoint Solves for Inverse Problems Governed by PDEs

Second-order, Newton-like algorithms exhibit convergence properties superior to gradient-based or derivative-free optimization algorithms. However, deriving and computing second-order derivatives needed for the Hessian-vector product in a Krylov iteration for the Newton step often is not trivial. Second-order adjoints provide a systematic and efficient tool to derive second derivative information. In this talk we show that the efficiency of an inexact Newton-CG approach to solve inverse problems governed by partial differential-based forward models can be improved with inexact Hessian-vector products using approximate second-order adjoint solves. We show numerical results for an inverse problem governed by an elliptic PDE, which reveal that close to the solution of the inverse problem, the tolerance of the second-order adjoint solves can be relaxed, which leads to reducing the number of inner Krylov iterations.

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CP3

Applying PDE Constrained Topology Optimization Methods to Optimal District Heating Network Design

Being able to integrate a variety of renewable and low-carbon energy sources, District Heating Networks (DHNs) are an important driver of the energy transition in the heating sector. Low network temperatures and fluctuating characteristics of renewable heat sources make it crucial to design optimal networks based on an accurate non-linear representation of the heat transport problem. To cope with this complexity of modern DHNs, their design and topology is commonly optimized solving a MILP or MINLP with classic combinatorial optimization methods. To overcome the loss of detail intrinsic to MILP and the limits on the problem scale for MINLPs, we present an adjoint gradient based approach to DHN optimization. This approach is inspired by well-established methods in the field of PDE constraint topology optimization. We reduce the amount of optimization variables to the set of design variables by solving the full nonlinear coupled flow- and heat transfer problem and computing adjoint gradients. To enforce discrete pipe design, we penalize cost and material properties of intermediate pipe diameters comparable to e.g. SIMP and ordered SIMP methods. We discuss the merits and challenges of applying different penalization methods to optimal DHN topology. Optimizing DHN topology requires to satisfy a big number of additional non-linear constraints. To maintain the scalability of the adjoint gradient calculation, we integrate this constraints using an Augmented Lagrangian approach.

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CP4

Optimization of Open-Loop Shallow Geothermal Systems Using the Adjoint Approach

Groundwater temperature directly affects the efficiency of groundwater heat pumps, also known as open-loop shallow geothermal systems. On the other side, groundwater heat pumps cause thermal anomalies in the groundwater, which can reach neighboring systems and deteriorate their operation. Therefore, it is important to optimally position these systems to avoid negative interactions and maximize overall efficiency. Flow and heat transport in porous media can be used to describe the influences of open-loop systems numerically. The processes are described with a system of nonlinear coupled PDEs. In addition, source/sink terms, representing extraction and injection wells, are modeled by non-smooth delta functions. The underlying problem is a PDE-constrained optimization problem including control (spatial coordinates of wells) and state (groundwater temperature) constraints. In this talk, we introduce an adjoint-based approach to solve this non-smooth PDE-constrained optimization problem. Dirac delta functions are approximated with smooth bump functions, which decouples source points from the mesh and enables computation of gradients. Nonlinear state constraints are incorporated using Moreau-Yosida type regularization terms. Spatial and temporal discretization, including meshing strategies, are analyzed as well. The approach is applied on real case scenarios with different numbers of heat pumps.

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CP4

A Rigorous Mathematical Method for Optimal Inventory Policies with Backlog Sales

This article is concerned with stochastic inventory control problems with backlog sales in stockout situations. We examine an infinite horizon model for piecewise linear concave ordering costs. Unlike finite horizons, however, infinite horizons lead to a functional equation for the value function. Such functional equations are solved numerically. Here we give a rigorous theory that explicitly solves this functional equation. We consider both the scenario in which an optimal selection can be made among two suppliers, as well as the scenario in which inventory can be purchased with incremental quantity discounts from a single supplier. We provide conditions that guarantee the optimality of the standard (s,S) policy. Moreover, when these conditions fail to hold, we show that an extended four-parameter policy is optimal.

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CP4

Multi-Fidelity Parallel Simulated Annealing Algorithm for Constrained Nuclear Fuel Cycle Optimization

A multi-fidelity parallel simulated annealing algorithm is proposed for solving a class of constrained combinatorial optimization problems in the application of design optimization for nuclear reactor cores. Solving these combinatorial problems is difficult due to the high dimensional design space, the non-smooth objective function and constraints, and, most importantly, expensive objective function and constraint evaluations that involve high-fidelity reactor simulations. While the existing parallel simulated annealing algorithm has been applied to solving high dimensional, non-smooth reactor optimization problems, the application to large scale problems is still hindered by the expensive objective function. The proposed algorithm aims to accelerate the optimization process by incorporating the parallel simulated annealing algorithm into a multi-fidelity framework, in which a low-fidelity, inexpensive reduced-physics model is used in the Markov Chain Monte Carlo sampler to speed up the exploration the feasible set and to guide the high-fidelity simulations. The low-fidelity model is adaptively refined in the course of the optimization by constructing a data-driven correction term using the high-fidelity simulation data. The combination of the parallel simulated annealing algorithm and the multi-fidelity modeling framework allows for efficient solution of large scale reactor core optimization problems and could benefit other scientific applications.

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CP4

Convergence Analysis of a Real-Time Distributed Control Algorithm for Radial Power Distribution Systems

The optimal power flow (OPF) problem optimizes a network-level objective function subject to the power distribution system's operating constraints. The large-scale integration of distributed energy resources (DERs) poses significant computational challenges to traditional OPF methods due to nonlinear power flow equations and communication delays leading to infeasible intermediate solutions. We present new distributed real-time approaches that optimize the objective while providing the voltage control and bounding communication delays. The Equivalence of Network-based Distributed Controller for Optimization (ENDiCo) algorithm is developed to achieve the network-level optimal solutions in fewer time steps by exploring the radial topology of the network based on the equivalence assumption. We present theoretical local and global convergence guarantees for the ENDiCo control algorithm. For the nonlinear model, the method of Lagrangian multipliers is used to prove the local convergence of every single agent at each time step for a specified range of parameters where KKT conditions are shown to hold. We further verify convergence numerically for specific parameter values within this range that are commonly used in practice. We also present rates of convergence of the algorithm using a combination of theoretical and numerical analysis. Finally, we prove global convergence for the agent communication case using the boundary of a small equivalent distribution system.

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CP4

A Lexicographic Column Generation Algorithm for Optimized Intra-Hospital Logistics

In this talk a solution algorithm is developed to dispatch transport orders to employees in hospitals and comparable institutions. This type of application problem may have several different optimization goals that are difficult to compare or convert to each other. In our case, the task is to compute an optimal transportation plan with respect to some hierarchical objective function including economic and ergonomic factors. For this purpose, a lexicographic optimization approach was coupled with a column generation method based on an enumerative branch-and-bound pricing algorithm to solve this vehicle routing problem. In order to achieve fast convergence, special pruning methods for the branch-and-bound search tree were developed to shorten the runtime of the enumeration process. In addition, the special structure of the lexicographic approach was exploited to further accelerate the column generation algorithm. Furthermore the solution method was evaluated using real-world data from several european clinics. The computational study shows that the newly developed algorithm can deliver high-quality results in most cases even optimal solutions within a short time. In addition, it significantly outperforms both a standard mixed-integer programming solver as well as the heuristics currently used by our industrial partner.

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CP4

Derivative-Free Mixed Binary Necklace Optimization for Cyclic-Symmetry Optimal Design Problems

We present an adapted trust-region method for solving computationally expensive black-box optimization problems with mixed binary variables that involve a cyclic symmetry property. This method is based on two main steps: successive continuous quadratic sub-problems and mixed binary quadratic sub-problems that both rely on interpolation models defined for mixed variables, valid within an adaptive trust region. To force exploration for binary variables, a no-good cut constraint is added to force the algorithm to explore outside of the previously explored regions. To deal with the cyclic symmetry, we introduce the necklace concept to define a distance that can avoid costly black-box objective-function evaluations at equivalent solutions. A theoretical proof of the local convergence of the adapted method is provided, based on simple reformulations of the sub-problems. Additionally, a new method for design of experiments in the mixed space is presented in order to choose scattered initial points for optimization. We generalize the approach based on kernel-embedding of probability to mixed discrete variables. Prior information on the problem, cyclic symmetry in our case, is introduced by the choice of an appropriate positive definite kernel. Several applications will be presented for a benchmark of functions and a simplified version of a turbine blade design application and compared with the state-of-the-art black-box optimization methods NOMAD and RBFopt.

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CP5

Concave Programming for ReLU-Based Neural Networks

Consider one layer $z = Wx+b, y = f(z)$ of a neural network with ReLU activation function for each vector component $f(z) = max(0, z)$. In a rather abstract setting (without a loss function and convolutional layers) one can determine W, b (for a given set of inputs x and outputs y) by solving the system of nonlinear equations $y = max(0, z)$ together with linear equalities $z = Wx + b$. Note that the max function is convex. Therefore, the solution set is on the boundary of a convex set defined by inequalities $max(0, z) - y \leq 0$. Using the summation of the left-hand-side expressions in these inequalities (proposed in e.g. V.P. Bulatov, O.V. Khamisov, Proc. of the 2nd SEI-IPRI Seminar On methods for solving the problems on energy power system development and control, pp. 90-95, 1992) we arrive to a concave programming problem with solutions given by maximization of a convex nonsmooth function over the set of linear constraints. The sum of max functions is a polyhedral function and a solution can be computed using linear programming, although finding this sum is prohibitively complex. We apply to this problem the modified conditions for global optimality, first proposed by A.S. Strekalovsky (see e.g. J.B. Hiriart-Urruty and Y.S. Ledyaev, “Note on the characterization of the global maxima of a (tangentially) convex function over a convex set”, Journal of Convex Analysis, Vol. 3, No. 1, pp. 55-61, 1996).

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CP5

A New Approach to High Contrast and Resolution Reconstruction in Quantitative Photoacoustic Tomography

A new framework for reconstruction of optical diffusion and absorption coefficients in quantitative photoacoustic tomography is presented. This framework comprises of a partial differential equation constrained optimization problem and the use of a relation between the diffusion and absorption coefficients that allow to obtain superior reconstructions. Further, a robust and fast sequential quadratic Hamiltonian scheme based on the Pontryagin's maximum principle (PMP) is used to solve for the optical coefficients. Results of several numerical experiments demonstrate that the proposed computational strategy is able to obtain reconstructions of the optical coefficients with high contrast and resolution for a wide variety of objects.

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CP5

Simultaneous Optimal Stratification and Allocation

The use of a stratified random sample is well known in modern sample survey, for example, in the census problem or in business statistics. The division of the entire population into meaningful groups is of central importance here. The aim of using such a stratification is to minimize the variance of the estimator for the variable of interest. In connection with the census problem this variable of interest is usually represented by the total population size and estimated by auxiliary data like registered persons in address size classes in the central register. For a high correlation between the auxiliary data and the variable of interest it is possible to stratify the auxiliary data to increase the efficiency of the estimator for the variable of interest. Based on this method it is also important to allocate the total sample size to each strata in order to get a representative result for the variable of interest. In my presentation I will introduce a block-coordinate descent method to find and optimal stratification as well as an optimal allocation simultaneously and show some preliminary results.

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CP5

A Recursive Multilevel Algorithm for Deep Learning

Neural networks are one of the most popular approaches in machine learning. They have been applied in many different scenarios like image classification or voice recognition. As computing capacity advances in modern computers, the complexity of neural networks also increases leading to deep networks. This entails the challenge of finding more efficient learning algorithms. In this talk, we formulate residual neural networks as discretisations of an Euler forward method. Motivated by this formulation, we explore measures to enhance the stability of residual neural networks. Moreover, we propose a recursive multilevel optimisation approach for training residual neural networks for image recognition by alternating training of networks on a coarse and on a fine dataset. We present numerical results to demonstrate the usefulness of our approach.

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CP5

Efficient Statistical Model Selection Framework for High-Dimensional Reaction-Diffusion Systems

We propose a novel computational framework for efficient high-dimensional parameter space characterization of reaction-diffusion models in systems biology. The method leverages the Lp-Adaptation algorithm, an adaptive-proposal statistical method for approximate high-dimensional design centering and robustness estimation. Today, access to unprecedented quality biological data allows us to build and test biochemically accurate reaction-diffusion models of intracellular processes. However, any increase in model complexity increases the number of unknown parameters and the computational cost of model analysis. To efficiently characterize the behavior and robustness of models with many unknown parameters is, therefore, a key challenge in systems biology. Our method is based on an oracle function, which describes for each point in parameter space whether the corresponding model fulfills given specifications. We propose specific oracles to estimate four parameter-space characteristics: bistability, instability, capability for pattern formation and for pattern maintenance. We benchmark the method and demonstrate that it allows exploring the capability of a model to undergo pattern-forming instabilities and to quantify model robustness for model selection in polynomial time with dimensionality. We present an application of the proposed method to inferring molecular mechanisms of pattern formation on intracellular membranes, that potentially drive self-organization in these systems.

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CP5

Reconstructing Functions from Nonlinear Observations

We consider nonlinear recovery problems which have traditionally been approached with nonconvex minimization methods. We show that, in many instances, these recovery tasks involve observations which can be represented using firmly nonexpansive operators, even when the original process is discontinuous. This allows our formulation to be recast in terms of a common fixed point problem, which is tractable with efficient and provenly-convergent algorithms. We present a new block-iterative algorithm for solving the best-approximation variant of this problem, along with numerical examples in signal and image processing.

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CP6

Algebraic Multigrid Barrier Method for Topology Optimization on Unstructured Meshes

Academic examples of topology optimization are often based on simple design domains that can be discretized by structured meshes. For large-scale problems, where the efficient solution of linear systems becomes increasingly important, this facilitates the use of geometric multigrid (MG) methods. However, non-trivial design domains generally necessitate the use of unstructured meshes. This, in turn, requires switching to algebraic MG methods, such as the smoothed aggregation (SA) method, introduced by Vaněk et al. in 1995. Building on previous work, we apply a penalty-barrier multiplier method to large-scale minimum compliance topology optimization problems, solving the arising linear systems by an SA-MG preconditioned MINRES solver. As the system matrix changes at every iteration, different SA strategies for computing the prolongation operators required for the MG method are employed. We compare these in terms of overall number of iterations as well as overall time needed to solve the optimization problem.

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CP6

Simulation Based Optimization of Multiphase Flow

In this talk, we present a simulation based optimization approach for optimal control of multiphase flow in the context of wetting phenomena. In general, the mathematical model of multiphase flow is governed by the Navier-Stokes equations together with jump conditions to connect the flow of the different fluids or phases at their interfaces. Based on L_p-maximal regularity of the underlying linear twophase problem we show the differentiability of the solution with respect to initial and distributed controls for appropriate spaces. To describe dynamic wetting or dewetting, the Navier-Stokes Equations are complemented by a transport equation for flow advection. This transport equation originates from an algebraic Volume-of-Fluid approach, that leads to an One-Field-Formulation of the problem. We use the introduced model for the simulation and optimization of a wetting process, motivated by gravure printing. For good printing results, it is essential to remove excess ink from the printing plate, except for a thin film that remains. For this purpose, a steel strap is pulled over the surface, which is also called a doctor blade. Our aim is to develop a gradient-based multilevel optimization method for shape optimization of the doctor blade and parameter identification problems arising in wetting processes. To achieve this, we derive sensitivity equations for the continuous flow problem together with a suitable descretization procedure. Furthermore, we show numerical results.

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CP6

Use of Topology Optimization to Improve the Energy Storage Capacity of Flywheels for Grid-Scale Energy Storage

The energy storage capacity of flywheels used for short duration grid energy storage functions, like power quality and voltage support, can be improved by optimizing the geometry of the flywheel rotor. Low speed flywheel rotors made from isotropic materials, such as steel, have a low cost of energy storage compared to high-speed composite flywheels and can be manufactured with complex geometries. It is hypothesized that the use of topology optimized rotors can reduce material costs and improve the specific energy of the device. In this contribution, a stress-constrained topology optimization framework to determine the best 2D rotor topology to maximize the energy capacity of the flywheel at varying operating speeds is developed. The flywheel is subject to a local volume fraction constraint to limit the amount of material used while ensuring connectivity between the shaft and the rim. An aggregated relaxed stress constraint is used to avoid material failure. A density filtering technique, along with a projection filter, ensures convergence of the topology to a discrete design without chequerboard patterns. Results from the developed framework will aim at showing the possible gains in specific energy by comparing the performance of topologically optimized rotors to state-of-the-art designs. The total cost of rotor material is also expected to reduce as the specific energy increases.

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CP6

Consistency of a Phase Field Regularisation for An Inverse Problem Governed by a Quasilinear Maxwell System

We tackle an inverse problem of reconstructing a discontinuous coefficient in quasilinear H(curl) magnetostatic equations from measurements in a subdomain. To overcome the ill-posedness of the inverse problem, we investigate two regularisations posed as constrained minimisation problems. The first involves perimeter penalisation and the second involves phase field regularisation. Existence of minimisers and consistency as the penalisation parameters tending to zero are discussed. We show under ideal situations a relation between parameters that allows one to obtain a solution to the inverse problem from the phase field solutions. Then, we investigate the convergence of the first order optimality conditions of the phase field problem to the optimal conditions obtained from shape calculus, leading to a necessary optimality system for the perimeter regularised problem. This is joint work with Irwin Yousept.

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CP6

Detection of Model Uncertainty in the Dynamic Linear-Elastic Model of Vibrations in a Truss

Dynamic processes have always been of profound interest for scientists and engineers alike. Often, the mathematical models used to describe and predict time-variant phenomena are uncertain in the sense that governing relations between model parameters, state variables and the time domain are incomplete. In this talk we present an algorithm for the detection of model uncertainty which combines parameter estimation, optimum experimental design and classical hypothesis testing within a probabilistic frequentist framework. The best setup of an experiment is defined by optimal sensor positions and optimal input configurations which both are the solution of a PDE-constrained optimization problem. The data collected by this optimized experiment then leads to variance-minimal parameter estimates. We develop efficient adjoint-based methods to solve this optimization problem with SQP-type solvers. The crucial test which a model has to pass is conducted over the claimed true values of the model parameters which are estimated from pairwise distinct data sets. For this hypothesis test, we divide the data into k equally-sized parts and follow a k-fold cross-validation procedure. We demonstrate the success of our approach in simulated experiments with a vibrating linear-elastic truss.

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CP7

Machine Learning Directed Optimization for Force Fields

In this work, we propose a machine learning directed optimization framework to tune classical molecular simulation force fields. We find that our surrogate-assisted optimization approach, which integrates Gaussian process surrogate models and support vector machine classifiers, facilitates rapid tuning of force fields and provides a quick and efficient route to accurate, physics-based molecular models. In our case studies, we tune van der Waals repulsion-dispersion interaction parameters to reproduce experimental property measurements. In our first demonstration case, we optimize force fields for two hydrofluorocarbons, HFC-32 and HFC-125, for liquid and vapor densities, vapor pressures, and enthalpies of vaporization. We can find 4 HFC-32 and 4 HFC-125 force field parameter sets in a time-frame of weeks which give less than 1.5% and 2.5% mean absolute percent error, respectively, in all of the properties of interest. Additionally, we find that these parameter sets are able to predict transport and critical properties accurately for HFC-32 and HFC-125 without further tuning. In our second demonstration case, we apply our framework to develop a force field to predict solid properties of ammonium perchlorate, including lattice parameters, unit cell structure, and hydrogen bond distances, angles, and symmetry. Multiple parameter sets have been found that outperform existing force fields in reproducing experimental observations of the listed quantities.

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CP7

Recognizing Staircase Compatibility on a Subclass of m-Partite Graphs

For the problem to find an m-clique in an m-partite graph staircase compatibility is a polynominal-time solvable subcase. It has been successfully applied to improve solvability of railway timetabling problems, where it appears as a central subproblem. Staircase compatibility is a property of an m-partite graph together with total orders on the subsets of the graph partition, and allows for efficiently solvable totally unimodular linear programming formulations. Our work focuses on determining the required total orders if the partition is known, but the orders are yet to be determined. This opens up the possibility to apply these formulations to applications where the orders are not given canonically. Although the problem is $\mathcal{NP}$-hard in the general case, we can prove polynominal computability of the required total orders for bipartite graphs as well as a subcase of m-partite graphs by providing polynomial-time algorithms. To empirically demonstrate the efficiency of our algorithm for m-partite graphs, we evaluate its performance on a set of artificial instances as well as real-world instances from a railway timetabling application. For the real-world instances it showed, that applying our ordering-algorithm and subsequently solving the problem via the aforementioned totally unimodular formulations indeed outperforms a generic formulation that does not exploit staircase compatibility.

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CP7

The Non-Stop Disjoint Trajectories Problem

Given an undirected network with traversal times on its edges and connection requests from sources to destinations for commodities with release dates. The non-stop disjoint trajectories problem is to find trajectories that fulfill all requests, such that the commodities never meet. In this extension to the NP-complete disjoint paths problem, trajectories must satisfy a non-stop condition, which disallows waiting at vertices or along arcs. This problem variant appears, for example, when disjoint aircraft trajectories shall be determined. We study the complexity of feasibility and optimization on three graph classes that are frequently used where space and time are discretized simultaneously: the path, the grid, and the mesh. We show that if all commodities have a common release date, feasibility can be decided in polynomial time on paths. For the unbounded mesh and unit-costs, we show how to construct optimal trajectories. In contrast, if commodities have individual release intervals and restricted turning abilities, then feasibility on paths is NP-complete. For the mesh and arbitrary edge costs, with individual release dates and restricted turning abilities of commodities, we show that optimization and approximation are not fixed-parameter tractable. This is joint work with Frauke Liers, Sarah Neumann (both FAU Erlangen-Nuremberg, Germany) and Francisco Javier Zaragoza Martnez (Universidad Autnoma Metropolitana Azcapotzalco, Mexico).

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CP7

Efficient Use of the Quantum Linear System Algorithms in Interior Point Methods for Linear Optimization

Due to its potential to revolutionize computing, Quantum Computing (QC) has attracted significant interest. Mathematical optimization problems yield one of the most important classes of problems with widespread use in practice and intriguing computational challenges. After the publication of the HHL method for solving linear equation systems, Quantum Interior Point Methods (QIPMs), were proposed to solve Semi-definite Optimization, Linear Optimization, and Second-order Cone Optimization problems. Most of them have applied Quantum Linear Equation System (QLSA) solvers at each iteration of their algorithm. However, the use of QLSA solvers in QIPMs comes with many challenges, such as having ill-conditioned systems and the error of QLSAs, which must be addressed when combining classical Interior Point Methods and QLSA solvers. In this presentation, we discuss how one can use QLSAs in QIPMs efficiently. Accordingly, an inexact infeasible QIPM is developed to solve linear optimization problems. We also discuss how we can get an exact solution by Iterative Refinement without excessive time of QLSAs. We also implemented our quantum method and analyze it empirically by using quantum simulators.

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CP7

Tree Bounds for Sums of Bernoulli Random Variables: A Linear Optimization Approach

We study the problem of computing the tightest upper and lower bounds on the probability that the sum of n dependent Bernoulli random variables exceeds an integer k. Under knowledge of all pairs of bivariate distributions denoted by a complete graph, the bounds are NP-hard to compute. When the bivariate distributions are specified on a tree graph, we show that tight bounds are computable in polynomial time using a compact linear program. These bounds provide robust probability estimates when the assumption of conditional independence in a tree structured graphical model is violated. We demonstrate, through numericals, the computational advantage of our compact linear program over alternate approaches. A comparison of bounds under various knowledge assumptions such as univariate information and conditional independence is provided. An application is illustrated in the context of Chow Liu trees, wherein our bounds distinguish between various trees which encode the maximum possible mutual information.

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CP7

Multifacility Location Problems Based on Mixed Integer Programming

The talk introduces a new approach to solve multifacility location problems based on mixed integer programming and algorithms for minimizing differences of convex (DC) functions. This class of multifacility location problems is very difficult to solve because of its intrinsic discrete, nonconvex, and nondifferentiable nature. We first reformulate the problem under consideration as a continuous optimization problem then develop a new DC type algorithm involving Nesterov's smoothing. We also implement our method with MATLAB, numerical tests are done on both artificial and real data sets.

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CP8

A Gradient Descent Akin Method for Inequality Constrained Optimization

We propose a gradient descent akin method for solving inequality constrained optimization problems: at each iteration, we compute a search direction using a linear combination of the negative and normalized objective and constraint gradient. The method is derived from our previous work, a modified search direction inspired by the singular value decomposition. Our research interest has been in the theory of the method, and some of the results can be found in [Chen et al., arXiv: 1902.04040, 2020]. Using a dynamical systems perspective, we show some of the asymptotic global and local behaviors of the method. Specifically, the method is globally convergent to local minimizers, provided that all saddle points are strict. Computational experiments in large-scale shape optimizations show that the method is robust.

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CP8

A Block Coordinate Descent Method for Sensor Network Localization

The problem of sensor network localization (SNL) can be formulated as a semidefinite programming problem with a rank constraint. We propose a new method for solving such SNL problems. We factorize a semidefinite matrix with the rank constraint into a product of two matrices via the Burer–Monteiro factorization. Then, we add the difference of the two matrices, with a penalty parameter, to the objective function, thereby reformulating SNL as an unconstrained multiconvex optimization problem, to which we apply the block coordinate descent method. In this study, we also provide theoretical analyses of the proposed method and show that each subproblem that is solved sequentially by the block coordinate descent method can also be solved analytically, with the sequence generated by our proposed algorithm converging to a stationary point of the objective function. We also give a range of the penalty parameter for which the two matrices used in the factorization agree at any accumulation point and point out the relationship between the objective function of the reformulated problem and the augmented Lagrangian. Numerical experiments confirm that the proposed method does inherit the rank constraint and that it estimates sensor positions faster than other methods without sacrificing the estimation accuracy, especially when the measured distances contain errors. In addition, the results show that our method does not run out of memory even for large-scale SNL problems.

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CP8

Stochastic Compositional Gradient Descent under Compositional Constraints

This work studies constrained stochastic optimization problems where the objective and constraint functions are convex and expressed as compositions of stochastic functions. The problem arises in the context of fair classification, fair regression, and the design of queuing systems. Of particular interest is the large-scale setting where an oracle provides the stochastic gradients of the constituent functions. The goal is to solve the problem with a minimal number of calls to the oracle. Owing to the compositional form, stochastic gradients provided by the oracle do not yield unbiased estimates of gradients. Instead, we construct approximate gradients by tracking the inner function evaluations, resulting in a quasi-gradient saddle point algorithm. We prove that the proposed algorithm finds optimal and feasible solution almost surely. We further establish that the proposed algorithm requires $\mathcal{O}(1/\epsilon^4)$ data samples to obtain an ϵ-approximate optimal point while also ensuring zero constraint violation. The result matches the sample complexity of the stochastic compositional gradient descent method for unconstrained problems and improves upon the best-known sample complexity results for the constrained settings. The efficacy of the proposed algorithm is tested on both fair classification and fair regression problems. The numerical results show that the proposed algorithm outperforms the state-of-the-art algorithms in terms of convergence rate.

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CP8

A Cone Decomposition Method for Semi-Integer Problems

In many optimization problems, a decision variable is mostly confined in continuous decision variables or in discrete decision variables. However, in various real-world applications, there are some cases that the decision variable should be confined in a disconnected set, that is, the feasible solution is either the lower bound or an integer in an inclusive range. However, such semi-integer variables are usually more challenging to solve than continuous variables. This talk will discuss the application of cone decomposition method (CDM), which is proposed based on a cutting plane method and a mathematical structure of the second order cones, to reduce computation time for solving a semi-integer problem arising from forest tree breeding. We will show some numerical results to compare the performance of CDM with and without outer approximation by employing different MILP solvers. Furthermore, we discuss the implementation of other cutting method to improve CDM performance. All of these implementations are not limited to the tree breeding problem, but they can also be used for solving other similar problems such as portfolio selection problem.

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CP8

On the Implementation of Multidimensional Searches into a Dual Simplex Solver and a Primal-Dual Interior Point Solver

The class of multidimensional search algorithms has received attention in the last years as a method to solve linear programs. Differently than the traditional one-dimensional search algorithms, these techniques search over the space of feasible solutions through multiple directions. For a simplex framework, this consists in pivoting multiple variables in the basis simultaneously at each iteration while for an interior point framework, multiple search directions determine the next interior solution at each step. This talk will present the implementation details of two and three-dimensional search methods into a dual simplex solver and a primal-dual interior point solver. For the first, HiGHS, an open-source solver for large-scale sparse linear programming is considered. For the second, PCx, an interior-point predictor-corrector linear programming solver is used. Computational results on benchmark linear programs will be presented as well some theoretical advancements in the methods to solve the subproblems of these algorithms.

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CP8

Global Convergence of a Stabilized Sequential Quadratic Semidefinite Programming Method for Nonlinear Semidefinite Programs Without Constraint Qualifications

In this presentation, we propose a new sequential quadratic semidefinite programming (SQSDP) method for solving nonlinear semidefinite programs (NSDPs), in which we produce iteration points by solving a sequence of stabilized quadratic semidefinite programming (QSDP) subproblems, which we derive from the minimax problem associated with the NSDP. Differently from the existing SQSDP methods, the proposed one allows us to solve those QSDP subproblems just approximately so as to ensure global convergence. One more remarkable point of the proposed method is that any constraint qualifications (CQs) are not required in the global convergence analysis. Specifically, under some assumptions without CQs, we prove the global convergence to a point satisfying any of the following: the stationary conditions for the feasibility problem; the approximate-Karush-Kuhn-Tucker (AKKT) conditions; the trace-AKKT conditions. The latter two conditions are the new optimality conditions for the NSDP presented by Andreani et al. (2018) in place of the Karush-Kuhn-Tucker conditions. Finally, we conduct some numerical experiments to examine the efficiency of the proposed method.

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CP9

On a Primal-Dual Newton Proximal Method for Convex Quadratic Programs

We introduce QPDO, a primal-dual method for convex quadratic programs which builds upon and weaves together the proximal point algorithm and a damped semismooth Newton's method. The outer proximal regularization yields a numerically stable method, and we interpret the proximal operator as the unconstrained minimization of the primal-dual proximal augmented Lagrangian function. This allows the inner Newton's scheme to exploit sparse symmetric linear solvers and multi-rank factorization updates. Moreover, the linear systems are always solvable independently from the problem data and exact linesearch can be performed. The proposed method can handle degenerate problems, provides a mechanism for infeasibility detection, and can exploit warm starting, while requiring only convexity. We present details of our open-source C implementation and report on numerical results against state-of-the-art solvers. QPDO proves to be a simple, robust, and efficient numerical method for convex quadratic programming.

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CP9

Iteration Complexity of a Proximal Augmented Lagrangian Method for Solving Nonconvex Composite Optimization Problems with Nonlinear Convex Constraints

This talk presents and analyzes a nonlinear inner accelerated proximal inexact augmented Lagrangian (NL-IAPIAL) method for solving smooth nonconvex composite optimization problems with nonlinear $\mathcal{K}$-convex constraints, i.e., the constraints are convex with respect to the order given by a closed convex cone $\mathcal{K}$. Each NL-IAPIAL iteration consists of inexactly solving a proximal augmented Lagrangian subproblem by an accelerated composite gradient (ACG) method followed by a Lagrange multiplier update. Under some mild assumptions, it is shown that NL-IAPIAL generates an approximate stationary solution of the constrained problem in $\mathcal{O}(\log(1/\rho)/\rho^3)$ ACG iterations, where $\rho > 0$ is a given tolerance. Numerical experiments are given to illustrate the computational efficiency of the presented method.

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CP9

Adaptive Hessian Initialization Strategy for L-Bfgs Solving Non-Linear Inverse Problems

Many inverse problems are treated as an optimization problem, where the objective function is a sum of a data-fitting term and a regularization. Often, the Hessian of data-fitting is computationally expensive. But, the regularizers Hessian is easy to compute. The L-BFGS scheme approximates Hessian based on an initial approximation and an update rule that models current local curvature information. The initial approximation significantly affects the scaling of a search direction and the overall convergence of the method. This talk discusses the various novel, simple, and effective Hessian initialization schemes. We replace the Hessian of the data-fitting with a scalar and keep the Hessian of the regularizer to re-initialize the Hessian at every iteration. The scalar satisfies the secant equation in the sense of ordinary and total least squares and geometric mean regression. We improve upon the secant-based schemes by tuning the scalar adaptively based on the recent line-search steps. Our new strategy not only leads to faster convergence, but the quality of the numerical solutions is generally superior to simple scaling based schemes. We also prove that the proposed scalar parameters are eigenvalue estimates of the Hessian of a data-fitting term. The implementation of our strategy requires only a small change of a standard L-BFGS code. Our experiments on convex quadratic problems and non-convex image registration problems confirm the effectiveness of the proposed approach.

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CP9

Sequential Quadratic Optimization for Nonlinear Optimization Problems on Riemannian Manifolds

We consider optimization problems on Riemannian manifolds with equality and inequality constraints, which we call Riemannian nonlinear optimization (RNLO) problems. Although they have numerous applications, the existing studies on them are limited especially in terms of algorithms. In this paper, we propose Riemannian sequential quadratic optimization (RSQO) that uses a line-search technique with an ℓ_1 penalty function as an extension of the standard SQO algorithm for constrained nonlinear optimization problems in Euclidean spaces to Riemannian manifolds. We prove its global convergence to a Karush-Kuhn-Tucker point of the RNLO problem by means of parallel transport and exponential mapping. Furthermore, we establish its local quadratic convergence by analyzing the relationship between sequences generated by RSQO and the Riemannian Newton method. Ours is the first algorithm that has both global and local convergence properties for constrained nonlinear optimization on Riemannian manifolds. Empirical results show that RSQO finds solutions more stably and with higher accuracy compared with the existing Riemannian penalty and augmented Lagrangian methods.

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CP9

An Accelerated Proximal Gradient Method for Multiobjective Optimization

In recent years, descent methods for multiobjective optimization problems have attracted much attention in the optimization community. For example, Fliege and Svaiter proposed the steepest descent method for differentiable multiobjective optimization problems. Afterward, a proximal gradient method, which can solve non-differentiable problems, was also considered. However, their accelerated versions are not sufficiently studied. Recently, El Moudden and El Mouatasim proposed a natural extension of Nesterovs accelerated method. They proved the global convergence rate of the algorithm $(O(1/k^2))$ under the assumption that the sequence of the Lagrangian multipliers of the subproblems is eventually fixed. However, this assumption is restrictive because it means that the method is regarded as the Nesterovs method for the weighting problem. In this work, we propose a new accelerated algorithm, in which we solve subproblems with terms that only appears in the multiobjective case. We also prove the proposed methods global convergence rate $(O(1/k^2))$ under a more natural assumption, using merit functions as a way to measure the complexity.

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CP9

Optimization Using Tunable Inexact Oracles

Simplicity of first-order methods makes their use widespread to solve many practical optimization problems. Recent works addressed the impact of inexact first-order information about the objective or inexact proximal steps in their convergence analysis, extending even further their field of applicability. In this work we highlight how both classical and accelerated Bregman Proximal Gradient algorithms rely on the ability, at each iteration, to ensure a common key decrease condition. We generalize existing results about the inexact counterpart of the above methods by relaxing this condition, combining both aforementioned sources of inexactness. As a byproduct we show that this generic relaxed condition also arises in the context of higher-order methods as the Inexact Tensor Method. We detail situations where the tightness of the condition above can be tuned upon demand, i.e. a more accurate first-order information about the objective or a more precise proximal step coming at the price of extra computations. We study optimal inexactness schedules for Bregman Proximal Gradient algorithms according to oracles' cost and a worst-case convergence analysis. Two optimality criteria, mutually dual, are investigated: ensuring a given primal accuracy at lowest possible cost and achieving the best primal accuracy at fixed computational budget. Our tunable approach mainly applies in the context of robust optimization, projection free optimization, relatively or non-smooth optimization.

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CP10

Duality Structure Gradient Descent: A First-Order Optimization Algorithm Based on a Coordinate-Wise Smoothness Assumption with Applications to Neural Nets

First-order optimization algorithms such as stochastic gradient descent are the method of choice for training machine learning models like neural networks. However, many non-asymptotic analyses of first-order algorithms involve assumptions like smoothness (that is, Lipschitz continuous gradients) or uniform bounds on variance that are too strong to hold for general neural nets. To address this we introduce an algorithm, named duality structure gradient descent (DSGD), that exploits a generalized "coordinate-wise" smoothness property that is satisfied by a large class of functions including multi-layer neural nets. DSGD can be viewed as a form of layer-wise coordinate descent, where at each iteration the algorithm greedily chooses one layer of the network to update, based on a rigorous lower bound on the possible improvement for each choice of layer. In the analysis, we bound the time required to reach approximate stationary points, and stationarity is measured in terms of a parameter-dependent family of norms that is derived from the network architecture.

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CP10

A Penalty Decomposition Approach for Multi-Objective Cardinality-Constrained Optimization Problems

We consider multi-objective optimization problems with a cardinality constraint on the vector of decision variables and additional linear constraints. For this class of problems, we analyze necessary and sufficient conditions of Pareto optimality. We afterwards propose a Penalty Decomposition type algorithm, exploiting multi-objective descent methods, to tackle the aforementioned family of problems. We conduct a rigorous convergence analysis for the proposed method, where we prove that the produced sequence of points has limit points, each one being feasible and satisfying first-order optimality conditions. Numerical computational experiments, carried out on instances of a relevant problem such as the mean/variance portfolio selection, in its multi-objective formulation with sparsity constraints, show that the proposed procedure is effective at finding solutions forming good Pareto sets approximations.

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CP10

A Dca for Mpccs Converging to a S-Stationary Point

This work deals with an Algorithm based on a DC decomposition (Difference of Convex functions) which solves MPCCs and we prove that it converges to a strongly stationary point under MPCC-LICQ. More precisely, we consider the following MPCC:

$$\begin{array}{ll} \min & f(w) \\ \text{subject to} & g(w) \leq 0 \;, h(w) = 0 \\ & 0 \leq y \perp z \geq 0. \end{array} \tag{1}$$

The functions g_i are supposed to be C^1 and convex on their domain, and h is supposed to be affine. We prove that under suitable assumptions, (1) can be formulated as a DC program. In this work, we relate the strong stationarity in MPCCs with the optimality conditions in DC programs, and use it in order to prove the convergence of the proposed algorithm based on a DC decomposition to a strong stationary point for MPCC under MPCC-LICQ. This work has been published in [M. Maréchal, A DCA for MPCCs converging to a S-stationary point, Pacific Journal on Optimization 16(3) (2020) 343-368], and it extends the results obtained in [F. Jara-Moroni, J. S. Pang and A. Wachter, A study of the difference-of-convex approach for solving linear programs with complementarity constraints, Mathematical Programming 169(1) (2018) 221-254]. We have done some numerical tests and the results obtained are consistent with the theoretical results we have demonstrated in this article.

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CP10

Nonlinear Primal-Dual Algorithms for Solving Sparse Logistic Regression Problems

Logistic regression is the most frequently used model in statistics to describe the relationship between a binary response variable and predictor variables in datasets. It is often used as a variable selection tool to identify important predictor variables in big datasets, whose number can range from hundreds of thousands to billions. This task typically amounts to constructing sparse solutions to logistic regression problems regularized by an l_1 norm, and such problems are called sparse logistic regression problems. Due to the sheer size of modern big datasets, solving sparse logistic regression problems depends on fast and scalable optimization algorithms. State-of-the-art algorithms for solving sparse logistic regression problems, however, either scale poorly with the size of datasets or only approximate solutions to these problems and may converge slowly at a suboptimal rate or fail to converge outright. As a result, solving large-scale sparse logistic regression problems remains challenging without access to adequate and costly computational resources. In this talk, we propose new nonlinear primal-dual algorithms for solving sparse logistic regression problems that address these shortcomings. We compare the performance of our algorithms to various state-of-the-art algorithms, including the coordinate based descent method implemented in the GLMNET package.

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CP10

A Vectorization Scheme for Robust Multiobjective Optimization Problems

In this talk, we consider a solution approach for set-based robust solutions to multiobjective optimization problems under uncertainty. Specifically, we derive a parametric family of (deterministic) semi-infinite multiobjective problems whose solution sets approximate, with desired accuracy, that of the original problem. The tractability of the semi-infinite constraints is also analyzed with tools of Fenchel duality. Our approach generalizes the standard epigraphical reformulation of robust scalar problems to the multiobjective setting.

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CP10

Uno: An Open-Source Framework for Unifying Nonlinear Optimization Methods

Iterative methods for nonlinear optimization usually share common ingredients, such as strategies to compute a descent direction or mechanisms that promote global convergence. Our new open-source framework for nonlinearly constrained optimization, UNO, offers a selection of off-the-shelf strategies that can be assembled at will. UNO thus unifies a variety of methods (e.g. trust-region filter SQP, line-search penalty Sℓ_1QP, line-search filter interior point method, ...) and interfaces with specialized solvers (BQPD, MA57) with no programming effort from the user. UNO also provides an interface to the algebraic modeling language AMPL. We present extensive results on a subset of problems from the CUTEst collection, and compare UNO against state-of-the-art solvers filterSQP, CONOPT, IPOPT, KNITRO, LANCELOT, LOQO, MINOS and SNOPT.

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CP11

On an Algorithm for Constrained Optimization Problems Given in Abs-Linear Form

The development of algorithms to optimize functions with constraints is an essential part of applied mathematics and of central importance for industrial applications. In an application context, it happens often that points exists where the objective functions and/or the constraints are not differentiable. In this talk we consider the solution of of pieceweise linear constrained optimization problems. For such problems the non-differentiabilty is frequently caused by an operator like the absolute value function. We exploit this structure by allowing constrained piecewise linear optimization problems to be represented by a matrix-vector based representation - the so-called Abs-Linear form. For problems given in the Abs-Linear form, we use a decomposition of the variable space into signature domains defined by the absolute value invocations. We also present a possible application of the algorithm in gas network optimization.

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CP11

Accelerating Inexact Successive Quadratic Approximation for Regularized Optimization Through Manifold Identification

For regularized optimization that minimizes the sum of a smooth term and a regularizer that promotes structured solutions, inexact proximal-Newton-type methods, or successive quadratic approximation (SQA) methods, are widely used for their superlinear convergence in terms of iterations. However, unlike the counter parts in smooth optimization, they suffer from lengthy running time in solving regularized subproblems because even approximate solutions cannot be computed easily, so their empirical time cost is not as impressive. In this work, we first show that for partly smooth regularizers, although general inexact solutions cannot identify the active manifold that makes the objective function smooth, approximate solutions generated by commonly-used subproblem solvers will identify this manifold, even with arbitrarily low solution precision. We then utilize this property to propose an improved SQA method, ISQA+, that switches to efficient smooth optimization methods after this manifold is identified. We show that for a wide class of degenerate solutions, ISQA+ possesses superlinear convergence not just only in iterations, but also in running time because the cost per iteration is bounded. In particular, our superlinear convergence result holds on problems satisfying a sharpness condition more general than that in existing literature. Experiments on real-world problems also confirm that ISQA+ greatly improves the state of the art for regularized optimization.

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CP11

An Inexact Proximal Difference-of-Convex Algorithm Based on Memoryless Quasi-Newton Methods

In this talk, we consider a class of difference-of-convex (DC) optimization problems such that the objective function is the sum of a smooth function with Lipschitz gradient, a proper closed convex function, and a continuous concave function. For solving such problems, several proximal DC algorithms have been proposed. To accelerate the algorithms, we incorporate the proximal mappings scaled by memoryless quasi-Newton matrices to a classical proximal DC algorithm and propose an inexact proximal DC algorithm based on memoryless quasi-Newton methods. Although usual proximal mappings can be easily obtained in some special cases, calculating the scaled proximal mappings needs to solve a subproblem by iterative methods. Because it is difficult or much expensive to compute the scaled proximal mappings exactly, we adopt an inexact rule in the inner iterations. To calculate the scaled proximal mapping more easily, we consider a one or two-dimensional system of semismooth equations arising in calculating the scaled proximal mapping. By solving inexactly the system by a semismooth Newton method, the scaled proximal mapping can be obtained efficiently. Finally, we present some numerical experiments to investigate the efficiency of the proposed method.

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CP11

Subgradient Smoothing Method for Nonsmooth Nonconvex Optimization

In this talk we present a method for solving an unconstrained nonsmooth nonconvex optimization problem. In this method, the subproblem for finding search directions is reduced to the unconstrained minimization of a smooth function. This is achieved by using subgradients computed in some neighborhood of a current iteration point and by formulating the search direction finding problem as the minimization of the convex piecewise linear function over the unit ball. The hyperbolic smoothing technique is applied to approximate the minimization problem by a sequence of smooth problems. The convergence of the proposed method is studied and its performance is evaluated using a set of nonsmooth optimization academic test problems. In addition, the method is implemented in GAMS and numerical results using different solvers from GAMS are reported. The proposed method is compared with a number of nonsmooth optimization methods.

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CP11

A Smoothing Technique for Difference-of-Convex (DC) Programs and Algorithmic Development

In this talk we consider the minimization of a difference-of-convex (DC) function with or without linear constraints. We first propose a new smooth approximation for a generic DC function by replacing both components with their Moreau envelopes. The resulting smooth approximation is shown to be Lipschitz differentiable with tractable gradient evaluation, and captures both local and global structures of the original DC function. We give sufficient conditions that ensure the level-boundedness of the smooth approximation. Consequently, the classic gradient descent method as well as its inexact variant converge on the smooth approximation with rate $\mathcal{O}(K^{-1/2})$, where K is the number of proximal evaluations of both components, and deliver a stationary point of the original DC function in the limit. Furthermore, when the minimization is explicitly constrained in an affine subspace, we combine the proposed smoothing technique with the augmented Lagrangian function and derive two variants of the augmented Lagrangian method (ALM), named LCDC-ALM, focusing on different structures of the DC function. We show that LCDC-ALM finds an ϵ-approximate stationary solution in $\mathcal{O}(\epsilon^{-2})$ iterations. Comparing to existing ALM algorithms designed for linearly constrained weakly convex minimization, the proposed LCDC-ALM can be applied to a broader class of problems where the objective contains a nonsmooth concave component.

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CP11

On the Linear Convergence to Weak/standard D-Stationary Points of Dca-Based Algorithms for Structured Nonsmooth Dc Programming

We consider a class of structured nonsmooth difference-of-convex minimization. We allow nonsmoothness in both the convex and concave components in the objective function, with a finite max structure in the concave part. Our focus is on algorithms that compute a (weak or standard) d(irectional)-stationary point as advocated in a recent work of Pang et al. in 2017. Our linear convergence results are based on direct generalizations of the assumptions of error bounds and separation of isocost surfaces proposed in the seminal work of Luo et al. in 1993, as well as one additional assumption of locally linear regularity regarding the intersection of certain stationary sets and dominance regions. An interesting by-product is to present a sharper characterization of the limit set of the basic algorithm proposed by Pang et. al., which fits between d-stationarity and global optimality. We also discuss sufficient conditions under which these assumptions hold. Finally, we provide several realistic and nontrivial statistical learning models where all assumptions hold.

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CP12

Non-Smooth Unadjusted Langevin Algorithms Via Forward-Backward Envelope

One of the major key tools in high-dimensional Bayesian learning is the sampling techniques from a posterior distribution. A combination of Markov chain Monte Carlo (MCMC) methods with continuous dynamical systems and continuous optimization offers a fast and robust sampling strategy. The unadjusted Langevin algorithm (ULA) and its variants have received much attention during the last decade. Traditionally, we consider the log-concave distribution as the target distribution, where the potential is Lipschitz smooth and strongly convex. In the Bayesian framework, the potential is the sum of two functions, where the first one stands for the log-likelihood and the second one indicates the log-prior probability distributions that can be non-smooth (e.g., Laplace distribution). As such, in this study, we assume that the potential is the sum of a smooth (non-convex) log-likelihood function and a (non-smooth) convex log-prior function. This class of functions can be smoothed by the so-called forward-backward envelope (FBE). Therefore, combining the FBE with the classical unadjusted Langevin algorithm leads to a sampling method for non-smooth potentials. Owing to Lipschitz smoothness and (strong) convexity of FBE under some mild assumptions, it is possible to provide asymptotic and non-asymptotic convergence analysis of this algorithm. Our numerical experiments on some applications illustrate the efficiency of the proposed algorithm.

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CP12

Small Errors in Zeroth Order Convex Optimization Are Imaginary

The vast majority of zeroth order optimization methods try to imitate first order methods via some approximation of the gradient. A common method is to sample objective function evaluations and rely on a certain smoothing parameter to control the approximation error. If the function evaluations are noise-free, then, the smaller the smoothing parameter, the smaller the error. We show that for the best part of zeroth order methods this smoothing parameter can however not be chosen arbitrarily small as numerical cancellation errors will dominate. Using classical tools from numerical differentiation we will propose a method which does allow for arbitrarily small errors while simultaneously attaining (sub)optimal convergence rates.

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CP12

On Benchmarking Numerical Methods for Constrained Global Optimization

Various aspects of benchmarking deterministic and stochastic constrained global optimization methods are considered in this talk. Several techniques for testing numerical global optimization algorithms are described with a particular focus on the recently proposed operational zones https://doi.org/10.1016/j.matcom.2016.05.006 and aggregated operational zones https://www.nature.com/articles/s41598-017-18940-4 . A new generator of constrained test problems is also presented which is based on the GKLS generator https://dl.acm.org/doi/10.1145/962437.962444 widely used in the global optimization literature. It extends the previous generation procedure from the box-constrained case to the case of nonlinear constraints. The user has the possibility to fix the difficulty of tests in an intuitive way by choosing several types of constraints. A detailed information (including the global solution) for each of tests is provided to the user.

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CP12

Moreau Envelope of Supremum Functions with Applications to Infinite and Stochastic Programming

In this paper, we investigate the Moreau envelope of the supremum of a family of convex, proper, and lower semicontinuous functions. Under mild assumptions, we prove that the Moreau envelope of a supremum is the supremum of Moreau envelopes, which allows us to approximate possibly nonsmooth supremum functions by smooth functions that are also the suprema of functions. Consequently, we propose and study approximated optimization problems from infinite and stochastic programming for which we obtain zero-duality results and optimality conditions without the verification of constraint qualification conditions.

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CP12

Riemannian Trust-Region Method for Gaussian Mixture Models

In this talk, we consider Gaussian Mixture Models that are widely spread in Data Science and Statistics. The data is modeled to follow a mixture of K Gaussian distributions and the optimization task therein lies in finding the optimal parameters of the Gaussians and the mixture components. This task is commonly solved by the Expectation-Maximization algorithm from computational statistics as the positive-definiteness constraint of covariance matrices makes standard nonlinear optimization algorithms hard to use. In an alternative approach, we exploit the geometric structure of positive definite matrices and use the concepts of optimization on manifolds. We reformulate the problem for this setting such that we can obtain faster algorithms. We present a Riemannian Newton Trust-Region method and show preliminary numerical results.

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CP13

Non-Euclidean Multi-block Proximal Alternating Linearized Minimization Algorithms for Nonsmooth Nonconvex Optimization

We introduce and analyze BPALM and A-BPALM , two multiblock proximal alternating linearized minimization algorithms using Bregman distances for solving structured nonconvex problems. The objective function is the sum of a multi-block relatively smooth function (i.e., relatively smooth by fixing all the blocks except one) and blocks separable (nonsmooth) nonconvex functions. The sequences generated by our algorithms are subsequentially convergent to critical points of the objective function, while they are globally convergent under the KL inequality assumption. Moreover, the rate of convergence is further analyzed for functions satisfying the Lojasiewiczs gradient inequality. We apply this framework to orthogonal nonnegative matrix factorization (ONMF) that satisfies all of our assumptions and the related subproblems are solved in closed forms. We finally report some numerical results confirming the theoretical foundations.

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CP13

OpReg-Boost: Learning to Accelerate Online Algorithms with Operator Regression

This paper presents a new regularization approach – termed OpReg-Boost – to boost the convergence and lessen the asymptotic error of online optimization and learning algorithms. In particular, the paper considers online algorithms for optimization problems with a time-varying (weakly) convex composite cost. For a given online algorithm, OpReg-Boost learns the closest algorithmic map that yields linear convergence; to this end, the learning procedure hinges on the concept of operator regression. We show how to formalize the operator regression problem and propose a computationally-efficient Peaceman-Rachford solver that exploits a closed-form solution of simple quadratically-constrained quadratic programs (QC-QPs). Simulation results showcase the superior properties of OpReg-Boost w.r.t. the more classical forward-backward algorithm, FISTA, and Anderson acceleration, and with respect to its close relative convex-regression-boost (CvxReg-Boost) which is also novel but less performing.

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CP13

Beyond Local Optimality Conditions: the Case of Maximizing a Convex Function

Traditionally, conditions under which a feasible solution of a convex optimization problem is identified as optimal are based on infinitesimal calculus: the analysis of functions through their behavior on a microlevel. Consequently, it is unable to provide *global* optimality conditions for nonconvex problems such as convex maximization. We suggest an intuitively appealing notion to identify globally optimal solutions: distance to the global *minimizer* of the objective function. Based on this idea, we develop a two-phase algorithm to solve convex maximization problems. First, we find, or approximate, the furthest point in the feasible set from the global minimizer. This is still a convex maximization problem, but for ellipsoidal feasible sets it can be solved efficiently. For other feasible sets, we elect to approximate the feasible set and continue with the furthest point in this approximation instead. Then, in the second phase, we use an alternating direction method initialized with this value that converges to at least a local maximum, which is a good candidate to be a global maximizer by virtue of being an improvement over the furthest point, a good candidate in its own right. The alternating direction method is highly tractable, as it only requires maximizing a linear function over the feasible set in each iteration. We demonstrate the performance of our algorithm on randomly generated instances and instances from the literature.

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CP13

A Limiting Analysis on Regularization of Ill-Conditioned SDP and Its Implication to Duality Theory

We consider primal-dual pairs of semidefinite programs and assume that they are ill-posed, i.e., both primal and dual are either weakly feasible or weakly infeasible. Under such circumstances, strong duality may break down and the primal and dual might have a nonzero duality gap. Nevertheless, there are arbitrary small perturbations to the problem data which makes the perturbed primal-dual pair strongly feasible thus zeroing the duality gap. In this talk, we conduct an asymptotic analysis of the optimal value as the perturbation is driven to zero. Specifically, we fix two positive definite matrices M_p, M_d, and add them to make the primal and dual problems strictly feasible. Then, we analyze the behavior of the optimal value of the perturbed problem when the perturbation is reduced to zero keeping their proportion, i.e., we consider the perturbation of the form tM_p and tM_d with $t = 1$ and reduce t to zero. No further assumptions such as compactness or constraint qualifications are ever made. It will be shown that the optimal value of the perturbed problem converges to a value between the primal and dual optimal values of the original problem. Finally, the analysis leads us to the relatively surprising consequence that the infeasible interior-point algorithms for SDP generates a sequence converging to a number between the primal and dual optimal values, even in the presence of a nonzero duality gap.

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CP13

Determination of Convex Functions Via Subgradients of Minimal Norm

We show, in Hilbert space setting, that any two convex proper lower semicontinuous functions bounded from below, for which the norm of their minimal subgradients coincide, they coincide up to a constant. Moreover, under classic boundary conditions, we provide the same results when the functions are continuous and defined over an open convex domain. These results show that for convex functions bounded from below, the slopes provide sufficient first-order information to determine the function up to a constant, giving a positive answer to the conjecture posed in Boulmezaoud et al. (SIAM J Optim 28(3):20492066, 2018).

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CP13

On Standard Quadratic Programs with Exact and Inexact Doubly Nonnegative Relaxations

The problem of minimizing a (nonconvex) quadratic form over the unit simplex, referred to as a standard quadratic program, admits an exact convex conic formulation over the computationally intractable cone of completely positive matrices. Replacing the intractable cone in this formulation by the larger but tractable cone of doubly nonnegative matrices, i.e., the cone of positive semidefinite and componentwise nonnegative matrices, one obtains the so-called doubly nonnegative relaxation, whose optimal value yields a lower bound on that of the original problem. We present a full algebraic characterization of the set of instances of standard quadratic programs that admit an exact doubly nonnegative relaxation. This characterization yields an algorithmic recipe for constructing such an instance. In addition, we explicitly identify three families of instances for which the doubly nonnegative relaxation is exact. We also provide an algebraic characterization of the set of instances for which the doubly nonnegative relaxation has a positive gap and show how to construct such an instance using this characterization.

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MS1

Large-Scale Linear Equality Constrained Optimization with Reduced Compact Representation

Large optimization problems with linear constraints $Ax = b$ have been used to formulate statistical and machine learning tasks. Computing search directions is the main challenge. When only gradient information is available, we estimate the Hessian matrix by a limited memory BFGS matrix. To handle the associated KKT system, we observe that the (1,1) block of the inverse KKT matrix is unchanged when projected onto the nullspace of A. Using this property, we develop a reduced compact representation (RCR) that decouples the computation of a search direction into an orthogonal projection and additional small terms. Orthogonal projections are computed using sparse QR of A^T and preconditioned LSQR. We implement the RCR in two trust-region algorithms. In numerical experiments on large problems, the proposed algorithms are more efficient, often significantly, compared to existing implementations.

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MS1

A Structured Modified Newton Approach for Solv-

ing Systems of Nonlinear Equations Arising in Interior-Point Methods for Quadratic Programming

We focus on interior-point methods for inequality-constrained quadratic programs, and particularly on the system of nonlinear equations to be solved at each iteration. Newton iterations give high quality solutions, but we seek modified Newton systems that are computationally less expensive at the expense of lower quality solutions. We propose a structured modified Newton approach where each modified Jacobian is composed of a previous Jacobian plus one low-rank update matrix per succeeding iteration. For a given rank, each update matrix is chosen to make the modified Jacobian closest to the current Jacobian in both 2-norm and Frobenius norm, while preserving the sparsity pattern of the Jacobian. Each modified Jacobian may be viewed as a Jacobian at a different point. The choice of update matrix is motivated by asymptotic results in an ideal theoretical framework. We give numerical results with a basic primal-dual interior-point implementation to investigate the practical performance within and beyond the theoretical framework. To improve performance, we motivate and construct two heuristics to be added to the method.

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MS1

Second-Derivative SQP Methods for Large-Scale Nonconvex Nonlinear Optimization

We present an SQP method that uses first and second derivatives of the problem functions and solves the QP subproblems with a shifted primal-dual interior method. The interior method can exploit a good starting point (it can be "warm-started"), and it implicitly regularizes the subproblem, ensuring convergence under weak assumptions on the problem. We discuss the treatment of infeasible and unbounded subproblems, and present numerical results on large nonconvex problems.

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MS1

Stochastic Gradient Descent Method with Bandwidth-Based Step Size

We investigate the stochastic gradient descent (SGD) method where the step size is given by a banded region instead of a fixed formula. The optimal convergence rate under mild conditions and large initial step size is proved. Our analysis provides comparable theoretical error bounds for SGD associated with a variety of step sizes. In addition, the convergence rates for some existing step size strategies, e.g., triangular policy and cosine-wave, can be revealed by our analytical framework under the boundary constraints. The bandwidth-based step size provides efficient and flexible step size selection in optimization. We also propose a $1/t$ up-down policy and give several non-monotonic step sizes. Numerical experiments demonstrate the efficiency and significant potential of the bandwidth-based step-size in many applications.

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MS2

Quasi-Newton Optimization Methods: Combining Multi-Secant with Symmetry

Solving complex root-finding problems is now a common situation in engineering. In most industrial applications, numerical methods helped to develop pieces of software that can simply be considered as a black box solving a problem based on given input variables. When such a black box is available, optimization is a logical next step. After defining some objective function, a new question arises: which value should be given to the variables in order to reach this objective? It is interesting to note that for root-finding problems, one important strategy in recent research and applications, in particular in interaction problems, is the use of multi-secant (or multi-points) Quasi-Newton methods. However, this strategy has been very little explored in the context of optimization where symmetrical methods (BFGS in the lead) are the most used. It can be shown that the multi-secant property and the symmetry are generally mutually exclusive [Quasi-Newton Methods Using Multiple Secant Equations, Schnabel 83]. Although, as multi-secant methods perform very well for root-finding problems, we are interested in the application of those methods in optimization. In order to tackle the stated general impossibility to develop a symmetric multi-secant Quasi-Newton update formula, we expose three strategies and give an overview of some of their recent results: data perturbation, penalized methods and alternating projections.

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MS2

Behavior of Quasi-Newton Methods for Unconstrained Quadratic Optimization Problems with Noisy Data

In this talk, we present specially designed quasi-Newton methods for solving quadratic optimization problems in a noisy frame-work, where there are errors in the data. The methods range from well-known deterministic methods, such as the BFGS method, to stochastic methods solving stochastic optimization problems associated with each iteration. We discuss the tradeoff between computational cost of each iteration and speed of convergence. We also present results on problems where several samples of the gradient may be obtained at each iteration.

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MS2

Modeling of Quasi-Newton Methods for Unconstrained Quadratic Optimization Problems with Noisy Data

In this talk, we consider unconstrained quadratic optimization. We consider quasi-Newton methods that are identical to the method of conjugate gradients in exact arithmetic. We now study the behavior of different such quasi-Newton methods in a noisy frame-work, where there are errors in the data. In particular, we propose methods for computing high-accuracy solutions, which are based on formulating and solving stochastic optimization problems associated with each iteration.

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MS2

A New Multipoint Secant Method with a Dense Initial Matrix

In this presentation, we discuss a new multipoint symmetric secant (MSS) that uses a dense initial matrix rather than a multiple of the identity initial matrix. We discuss the convergence analysis of the new method and compare the numerical results of applying the new method with the standard MSS, which uses a multiple of the identity initial matrix, on several problems from the CUTEst test problem set.

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MS3

Regularisation methods for Large Scale Optimization

An adaptive regularization algorithm (AR1pGN) for unconstrained nonlinear minimization is considered, which uses a model consisting of a Taylor expansion of arbitrary degree and regularization term involving a possibly non-smooth norm. It is shown that the non-smoothness of the norm does not affect the $O(\epsilon_1^{-(p+1)/p)})$ upper bound on evaluation complexity for finding first-order ϵ_1-approximate minimizers using p derivatives. It is also shown that, if $p = 2$, the bound of $O(\epsilon^{-3})$ evaluations for finding "second-order" ϵ-approximate minimizers still holds for a variant of AR1pGN named AR2GN, despite the possibly non-smooth nature of the regularization term. Moreover, the adaptation of the existing theory for handling the non-smoothness results in an interesting modification of the subproblem termination rules, leading to an even more compact complexity analysis. In particular, it is shown when the Newtons step is acceptable for an adaptive regularization method. The approximate minimization of quadratic polynomials regularized with non-smooth norms is then discussed, and a new approximate second-order necessary optimality condition is derived for this case. A specialized algorithm is then proposed to enforce first- and second-order conditions that are strong enough to ensure the existence of a suitable step in AR1pGN (when p = 2) and in AR2GN, and its iteration complexity is analyzed.

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MS3

Constrained and Unconstrained Optimization in the Presence of Noise

In the first part of the talk, we consider the solution of constrained and unconstrained optimization problems when only noisy evaluations of the functions, constraints, and their derivatives are available. We present theoretical results characterizing the achievable accuracy in the solution when employing classical methods adapted to handle noise. In the second part of the talk we focus on the noisy derivative-free setting and propose simple extensions of Gauss-Newton, L-BFGS and interior points that employ smoothed finite difference approximations. We argue that these methods are highly competitive and versatile.

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MS3

Inexact Proximal Methods with Subspace Acceleration for Sparse Problems

I discuss inexact proximal-gradient (PG) methods for solving sparse optimization problems such those problems using sparsity-inducing regularization (e.g., Lasso, group

Lasso, and latent group Lasso). Unlike the majority of related methods in the literature, we allow inexact PG calculations that are based on verifiable termination conditions. We also discuss enhanced second-order variants that integrate subspace acceleration over small dimensional subspaces, thus keeping the cost per iteration relatively low. Theoretical convergence results and numerical tests on various learning problems will be presented.

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MS3

SQP Methods for Equality Constrained Stochastic Optimization

Sequential quadratic optimization algorithms are proposed for solving smooth nonlinear optimization problems with equality constraints. The main focus is the case when the constraint functions are deterministic, but the objective function is stochastic. It is assumed in this setting that it is intractable to compute objective gradient values explicitly, although one can compute stochastic gradient estimates. We consider exact and inexact solves of the Newton-SQP system separately. For exact solves, we propose an adaptive stepsize selection scheme, since the objective is stochastic, for which it is assumed that line searches would be intractable. For inexact solves, we propose additional conditions for characterizing appropriate inexact subproblem solutions to address challenges resulting from the stochasticity in the objective function. Under reasonable assumptions, convergence in expectation are established for our proposed algorithms. The results of numerical experiments demonstrate the practical performance of our proposed techniques.

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MS4

Variance-Reduced Proximal and Splitting Schemes for Monotone Stochastic Generalized Equations

We consider monotone inclusion problems where the operators are expectation-valued. We propose two avenues for addressing uncertainty in the mapping. (i) Variance-reduced stochastic proximal point methods. We develop amongst the first variance-reduced stochastic proximal-point schemes that achieves optimal deterministic rates of convergence in terms of solving proximal-point problems, where we believe the rates for monotone regimes are amongst the first available. Our analysis reveals that the schemes achieve optimal sample-complexity in some regimes. The generated sequences are shown to be convergent to a solution in an almost-sure sense. It is worth emphasizing that the schemes do not rely on Lipschitzian assumptions on the map. (ii) Variance-reduced stochastic modified forward-backward splitting scheme. In constrained settings, we consider structured settings when the map can be decomposed into an expectation-valued map A and a maximal monotone map B with a tractable resolvent. Akin to (i), we show that the proposed schemes are equipped with a.s. convergence guarantees, linear (strongly monotone A) and $\mathcal{O}(1/k)$ (monotone A) rates of convergence while achieving optimal oracle complexity bounds. The rate statements in monotone regimes appear to be amongst the first. Furthermore, the schemes rely on weaker moment requirements on noise as well as allow for weakening unbiasedness requirements on oracles in strongly monotone regimes.

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MS4

Distributed Variable Sample-Size Gradient-response and Best-response Schemes for Stochastic Nash Equilibrium Problems

This talk considers a stochastic Nash equilibrium problem, where each player minimizes a composite objective being the sum of an expectation-valued smooth function and a nonsmooth convex function with an efficient prox-evaluation. Under suitable monotonicity assumptions on the pseudogradient, we propose a distributed variable sample-size proximal stochastic gradient-response scheme, where each player combines a variance reduced proximal gradient response with multiple consensus steps for learning the aggregate. Under a suitable contractive property associated with the proximal best-response (BR) map, we further design a distributed variable sample-size proximal BR scheme, where each player estimates the aggregate by a consensus update and then solves a sample-average BR problem. For both schemes, when the sample-size increases at a suitable geometric rate and the number of consensus steps increase with $k+1$, the iterates converge at a geometric rate while the iteration, oracle and communication complexity to obtain an ϵ-Nash equilibrium are respectively $\mathcal{O}(\ln(1/\epsilon))$, $\mathcal{O}(1/\epsilon)$, and $\mathcal{O}(\ln^2(1/\epsilon))$. We further explore the convergence properties when the sample-sizes and communication rounds increase at a polynomial rate. Finally, we present some preliminary numerics to provide empirical support for the rate and complexity statements.

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MS4

Stochastic Inertial Forward-Backward-Forward Splitting for Monotone Stochastic Inclusions in

Hilbert Spaces

We propose and analyze the convergence of a novel stochastic algorithm for monotone inclusions that are sum of a maximal monotone operator and a single-valued Lipschitz continuous operator. The algorithm we propose is a natural stochastic extension of the classical forwardbackward-forward method. A key novelty of our approach is the detailed study of relaxation and inertial effects in the algorithmic design. Following an online variance reduction strategy via a mini-batch approach we achieve optimal iteration and almost optimal oracle complexity estimates. In the strongly monotone case, we obtain linear convergence rates in terms of a gap function, based on the Fitzpatrick function. Numerical results on two-stage games and empirical risk minimization under the overlapping group Lasso illustrate the decisive advantages of our method compared to its close competitors, like the accelerated mirror-prox scheme.

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MS4

Approximation and Distributed Computation of Generalized Nash Equilibria with Uncertain Coupled Constraints

We design a distributed algorithm to seek generalized Nash equilibria with uncertain coupled constraints. It is hard to find the exact equilibria directly, because the parameters in the coupled constraint come from general convex sets, which may not have analytic expressions. To solve the problem, we first approximate general convex sets by inscribed polyhedrons and transform the approximate problem into a variational inequality by robust optimization. Then, with help of convex set geometry and metric spaces, we prove that the solution to the variational inequality induces an ε-generalized Nash equilibrium of the original game in the worst case. Furthermore, we propose a distributed algorithm to seek an ε-generalized Nash equilibrium, and show the convergence analysis with Lyapunov functions and variational inequalities. Finally, we illustrate the effectiveness of the distributed algorithm by a numerical example.

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MS5

Randomized DFO Methods for Fitting Numerical Physics Models

We address the calibration of a computationally expensive nuclear physics model for which derivative information with respect to the fit parameters is not readily available. Of particular interest is the performance of optimization-based training algorithms when dozens, rather than millions or more, of training data are available and when the expense of the model places limitations on the number of concurrent model evaluations that can be performed. As a case study, we consider the Fayans energy density functional model, which has characteristics similar to many model fitting and calibration problems in nuclear physics. We analyze hyperparameter tuning considerations and variability associated with stochastic optimization algorithms and illustrate considerations for tuning in different computational settings. Based on our results, we propose some novel extensions to existing methods.

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MS5

Lookahead Acquisition Functions for Finite-Horizon Time-Dependent1Bayesian Optimization: Application to Quantum Optimal Control

We propose a novel Bayesian method to solve the maximization of a time-dependent expensive-to-evaluate stochastic oracle. We are interested in the decision that maximizes the oracle at a finite time horizon, given a limited budget of noisy evaluations of the oracle that can be performed before the horizon. Our recursive two-step lookahead acquisition function for Bayesian optimization, makes nonmyopic decisions at every stage by maximizing the expected increase in a value function—defined by the user—of the oracle, evaluated at the horizon. Specifically, we propose a generalized two-step lookahead framework with customizable value functions and illustrate how lookahead versions of classic acquisition functions such as the Expected Improvement, Probability of Improvement and Upper Confidence Bound, can be obtained. We demonstrate the utility of our proposed approach on several carefully constructed synthetic cases and a real-world quantum optimal control problem.

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MS5

Large-Scale Derivative-Free Optimization using

Subspace Methods

In existing techniques for model-based derivative-free optimization, the computational cost of constructing local models and Lagrange polynomials can be high. As a result, these algorithms are not as suitable for large-scale problems as derivative-based methods. In this talk, I will discuss a model-based derivative-free algorithm based on exploration of random subspaces, its worst-case complexity bounds, and some numerical results.

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MS5

Bayesian Optimization for Noisy Functions

Bayesian optimization (BO) is an increasingly popular approach in stochastic simulation optimizations. Despite its successful applications, there remain several practical issues that have to be addressed. These include the nontrivial optimization of the inner acquisition function to find the future evaluation points, the over-exploitative behavior of some BO algorithms and the effective allocation of replications to evaluation points. In this work, we propose a new partition-based BO framework for stochastic simulations that helps to overcome these issues. We further provide convergence guarantees for this framework and illustrate its finite time performance with several numerical experiments.

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MS6

Stochastic Polyak Step-Size for SGD: An Adaptive Learning Rate for Fast Convergence

We propose a stochastic variant of the classical Polyak step-size (Polyak, 1987) commonly used in the subgradient method. Although computing the Polyak step-size requires knowledge of the optimal function values, this information is readily available for typical modern machine learning applications. Consequently, the proposed stochastic Polyak step-size (SPS) is an attractive choice for setting the learning rate for stochastic gradient descent (SGD). We provide theoretical convergence guarantees for SGD equipped with SPS in different settings, including strongly convex, convex and non-convex functions. Furthermore, our analysis results in novel convergence guarantees for SGD with a constant step-size. We show that SPS is particularly effective when training over-parameterized models capable of interpolating the training data. In this setting, we prove that SPS enables SGD to converge to the true solution at a fast rate without requiring the knowledge of any problem-dependent constants or additional computational overhead. We experimentally validate our theoretical results via extensive experiments on synthetic and real datasets. We demonstrate the strong performance of SGD with SPS compared to state-of-the-art optimization methods when training over-parameterized models.

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MS7

Forward-Backward Methods: New Results and Perspectives

Several relevant problems in a variety of different fields, such as signal and image processing and machine learning, are formulated as optimization problems. The recent research leads such variational models to be more and more accurate and very challenging from the numerical and theoretical point of view. Indeed, the objective function to be minimized may include nonsmooth and nonconvex terms, which are difficult to handle by optimization methods, which are required to have both reliable theoretical convergence properties and effective practical performances. Forward-backward methods are valid tools when the objective function is the sum of a smooth, possibly nonconvex term plus a convex, possibly nonsmooth function. The corresponding iteration requires the gradient of the smooth part and the evaluation of the proximity operator associated to the convex term. One of the main challenges, from both implementation and theoretical point of view, arises when the the proximity operator has to be computed in an inexact way. The aim of this talk is to illustrate new convergence results about forward-backward methods with inexact computation of the proximity operator, under the assumption that the objective function satisfies the Kurdyka-Lojasiewicz property. The strength of our approach is that its implementation results in algorithms with well established convergence guaranties, which are also well performing on several relevant applications.

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MS7

Ergodic Convergence Rates for Optimal Transport and Wasserstein Barycenter Problems

Optimal Transport (OT) and Wasserstein Barycenter (WB) problems play a central role in imaging, clustering, machine learning, and statistics. Sinkhorn's algorithm and Iterative Bregman Projections are classical methods that use entropic penalization to approximate ”-optimal solutions of OT and WB, respectively. Recently, traditional methods of convex optimization such as Accelerated Mirror Descent and Alternating Minimization have been proved to achieve convergence rates with a better dependence on ” than classical approaches. Following these ideas, we study OT and WB through standard non-linear first-order methods. As an immediate result, we obtain upper bounds for the duality-gap that interestingly matches the accelerated rates of recent approaches. The new algorithm is simple and does not require entropic penalization. We study several variants of the new method including a new regularization strategy that makes the computations very stable. Numerical experiments on synthetic and real datasets are provided.

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MS7

Adaptive Acceleration for First-order Methods

First-order operator splitting methods are ubiquitous among many fields through science and engineering, such as inverse problems, image processing, statistics, data science and machine learning, to name a few. In this talk, through the fixed-point sequence, I will first discuss a geometry property of first-order methods when applying to solve non-smooth optimization problems. Then I will discuss the limitation of current widely used inertial acceleration technique, and propose a trajectory following adaptive acceleration algorithm. Global convergence is established for the proposed acceleration scheme based on the perturbation of fixed-point iteration. Locally, connections between the acceleration scheme and the well studied vector extrapolation technique in the field of numerical analysis will be discussed, followed by acceleration guarantees of the proposed acceleration scheme. Numeric experiments on various first-order methods are provided to demonstrate the advantage of the proposed adaptive acceleration scheme.

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MS7

Convergence of the Proximal Gradient Algorithm in the Context of An Adjoint Mismatch

The proximal gradient algorithm is a popular iterative algorithm to deal with penalized least-squares minimization problems. Its simplicity and versatility allow one to embed nonsmooth penalties efficiently. In the context of inverse problems arising in signal and image processing, a major concern lies in the computational burden when implementing minimization algorithms. For instance, in tomographic image reconstruction, a bottleneck is the cost for applying the forward linear operator and its adjoint. Consequently, it often happens that these operators are approximated numerically, so that the adjoint property is no longer fulfilled. In this talk, we focus on the proximal gradient algorithm stability properties when such an adjoint mismatch arises. By making use of tools from convex analysis and fixed point theory, we establish conditions under which the algorithm can still converge to a fixed point. We provide bounds on the error between this point and the solution to the minimization problem. We illustrate the applicability of our theoretical results through numerical examples in the context of computed tomography.

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MS8

A Scalable Deterministic Global Optimization Algorithm for Clustering Problems

The minimum sum-of-squares clustering (MSSC) task, which can be treated as a Mixed Integer Second Order Cone Programming (MISOCP) problem, is rarely investigated in the literature through deterministic global optimization. One reason is that a classic branch and bound (BB) scheme needs to perform branching on all variables, and the number of variables increases linearly as the number of data samples. Therefore, state-of-the-art global solvers cannot solve clustering problems even with tens of data points. In this paper, we modelled the MSSC task as a two-stage optimization problem and proposed a tailed reduced-space BB algorithm. We also designed several approaches to construct lower and upper bounds at each node in the BB scheme. One key advantage of this reduced-space algorithm is that it only needs to perform branching on the centers of clusters to guarantee convergence, and the size of centers is independent of the number of data samples. Another critical property of this algorithm is that bounds can be computed by solving small-scale sample subproblems. These two properties enable our algorithm to be scalable to the dataset with hundreds or even thousands of data points for finding a global ϵ-optimal solution. We performed numerical experiments and compared our proposed algorithms with the off-the-shelf global optimal solvers and classical local optimal algorithms. The results reveal a strong performance and scalability of our algorithm.

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MS8

Optimal Study Design for Reducing Variances of Coefficient Estimators in Change-Point Model

In longitudinal studies, we measure the same variables at multiple time-points to track their change over time. The exact schedules of participants visits time are often predetermined to accommodate ease of project management and compliance. So, the standard design schedules those visits at equally spaced time intervals. However, this standard design does not provide the best power of studies and the best precision of model parameter estimators. In this paper, we propose an optimal study design to better study the accelerated cognitive decline of senior adults, where a broken-stick model is often applied. We formulate this optimal design problem on scheduling participants visiting into a high-dimensional optimization problem and derive its approximate solution. Based on this approximation, we propose a novel design of the visiting scheme that aims to maximize the power (i.e. reduce the variance of estimators). Using both simulation studies and evidence from real data, we demonstrate that our design outperforms the standard design when we have strong prior knowledge of the change-points. This novel design help researchers plan their longitudinal studies with improved power in detecting pattern change without collecting extra data. Also, this individual-level scheduling system helps monitor seniors' cognitive function and, therefore, benefits the development of personal level treatment for cognitive decline, which agrees with the trend of the health care system.

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MS9

On Complexity and Convergence of High-Order Coordinate Descent Algorithms

Coordinate descent methods with high-order regularized models for box-constrained minimization are introduced. High-order stationarity asymptotic convergence and first-order stationarity worst-case evaluation complexity bounds are established. The computer work that is necessary for obtaining first-order ε-stationarity with respect to the variables of each coordinate-descent block is $O(\varepsilon^{-(p+1)/p})$ whereas the computer work for getting first-order ε-stationarity with respect to all the variables simultaneously is $O(\varepsilon^{-(p+1)})$. Numerical examples involving multidimensional scaling problems are presented. The numerical performance of the methods is enhanced by means of coordinate-descent strategies for choosing initial points.

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MS9

New Viewpoints, Variants and Convergence Theory for Stochastic Polyak Stepsizes

I will use our recently developed subsampled Newton Raphson method to design some new stochastic variance reduced methods and shed light on some old methods. Newton Raphson is a method for solving nonlinear equations. Subsampled Newton Raphson is a new variant that requires only a subsample of the rows in each step. To design a new optimization method by using subsampled Newton Raphson, I will first rewrite our optimization problem as a system of nonlinear equations and then apply the subsampled Newton Raphson method. As a first example, I will show that SPS (Stochastic gradient descent with a Polyak Stepsize) is a special case of the subsampled Newton Raphson method. I will then change the representation of these nonlinear equations to design a new variance reduced version of the SPS method. All instantiations of the subsampled Newton Raphson method come complete with a global convergence guarantee under some new star-convex type assumptions. As such, I will give a new global convergence theory for SPS and the variance reduced version.

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MS9

On the Use of Inexact Restoration in Finite-Sum Minimization

Finite-sum minimization is a relevant problem in many contexts, such as classification in machine learning and sample average approximation of objective functions formulated as mathematical expectation. We address finite-sum minimization via trust-region methods where the models are of order one or two and random since subsampled functions and derivatives are employed. The issue of choosing the sample size for approximating functions and gradients is delicate and several strategies have been proposed in the literature. In this talk we discuss a new strategy where the sample sizes used for function and gradient estimates change dynamically along the iterations and are adjusted by a deterministic rule inspired by the inexact restoration method, firstly proposed by J.M. Martinez and E.A. Pilotta for constrained optimization. We provide the complexity analysis of our procedures and their numerical validation on a set of convex and nonconvex classification problems.

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MS9

Stochastic Variance Reduced Gradient Methods with Variable Learning Rate

First order stochastic optimization methods are effective tools for the minimization of problems arising in machine learning applications. Since they only require the computation of the gradient corresponding to either a single or a small number of training examples, their overall cost per iteration is low and they can be exploited with very large datasets. However, two drawbacks can be identified when using first order stochastic optimization algorithms: a strong dependency of the practical performance on the choice of the learning rate and, even for very regular objective functions, a poor convergence rate due to the large variance introduced by random sampling. We develop a first order stochastic method which mitigates these two aspects. As for the first issue, we propose to select the learning rate by adapting, to the stochastic framework, a limited memory strategy developed for deterministic first order schemes. Such technique allows to automatically and adaptively select the learning rate at each iteration and to give a local estimate of the inverse of the local Lipschitz constant of the objective function gradient. Secondly, to reduce the variance of the stochastic gradient, we employ an adaptive subsampling strategy which assures the descent feature in expectation of the stochastic gradient directions and only needs that the learning rate is properly bounded by the Lipschitz parameter at any iteration. An extensive numerical experimentation is carried out.

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MS10

Inexact Proximal Augmented Lagrangian Methods with Arbitrary Linearly Convergent Inner Solver for Composite Optimization

We propose an inexact proximal augmented Lagrangian framework with explicit inner problem termination rule for composite convex optimization problems. We consider arbitrary linearly convergent inner solver including in particular stochastic algorithms, making the resulting framework more scalable facing the ever-increasing problem dimension. Each subproblem is solved inexactly with an explicit and self-adaptive stopping criterion, without requiring to set an a priori target accuracy. When the primal and dual domain are bounded, our method achieves $O(1/\sqrt{\epsilon})$ and $O(1/\epsilon)$ complexity bound in terms of number of inner solver iterations, respectively for the strongly convex and non-strongly convex case. Without the boundedness assumption, only logarithm terms need to be added and the above two complexity bounds increase respectively to $\tilde{O}(1/\sqrt{\epsilon})$ and $\tilde{O}(1/\epsilon)$, which hold both for obtaining ϵ-optimal and ϵ-KKT solution. Within the general framework that we propose, we also obtain $\tilde{O}(1/\epsilon)$ and $\tilde{O}(1/\epsilon^2)$ complexity bounds under relative smoothness assumption on the differentiable component of the objective function. We show through theoretical analysis as well as numerical experiments the computational speedup possibly achieved by the use of randomized inner solvers for large-scale problems.

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MS11

A Stochastic Second Order Extra-Step Scheme for Nonsmooth Nonconvex Optimization

In this talk, we present a novel stochastic second order-type extra-step method for solving a class of nonsmooth nonconvex composite-type optimization problems. We assume that gradient information of the smooth part of the objective function can only be approximated via calling stochastic oracles. The proposed method combines stochastic higher order steps for an underlying prox-type fixed-point equation with additional stochastic proximal steps to guarantee convergence. Specifically, based on suitable bounds on the utilized step sizes, we establish global convergence to stationary points in expectation and derive complexity results. Moreover, we discuss a variant of our approach using a variance reduction technique and show that it enjoys better convergence properties. Finally, numerical comparisons on large-scale logistic regression problems and sparse deep learning are provided illustrating the efficiency of the stochastic second order-type method.

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MS11

THOR: Second-Order Optimization for Deep Neural Network

Inspired by K-FAC, we propose a Trace-Based HardwareDriven Layer-Oriented Natural Gradient Descent Computation method, called THOR, to speed up the secondorder optimization method in the real application models. Specifically, we gradually increase the update interval and use the matrix trace to determine which blocks of Fisher Information Matrix(FIM) need to be updated. Moreover, by resorting the power of hardware, we have designed a Hardware-driven approximation method for computing FIM to achieve better performance. In our experiments, the results show that training ResNet-50 on ImageNet with THOR only takes 66.7 minutes to achieve a top-1 accuracy of 75.9% under an 8 Ascend 910 environment with MindSpore, a new deep learning computing framework. THOR can only takes 2.7 minutes to 75.9% with 256 Ascend 910.

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MS11

Inexact Proximal Stochastic Second-Order Methods for Nonconvex Composite Optimization

In this paper, we propose a framework of Inexact Proximal Stochastic Second-order (IPSS) method for solving nonconvex optimization problems, whose objective function consists of an average of finitely many, possibly weakly, smooth functions and a convex but possibly nonsmooth function. At each iteration, IPSS inexactly solves a proximal subproblem constructed by using some positive definite matrix which could capture the second-order information of original problem. Proper tolerances are given for the subproblem solution in order to maintain global convergence and the desired overall complexity of the algorithm. Under mild conditions, we analyse the computational complexity related to the evaluations on the component gradient of the smooth function. We also investigate the number of evaluations of subgradient when using an iterative subgradient method to solve the subproblem. In addition, based on IPSS, we propose a linearly convergent algorithm under the proximal PolyakLojasiewicz condition. Finally, we extend the analysis to problems with weakly smooth function and obtain the computational complexity accordingly.

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MS11

NG+ : A Multi-Step Matrix-Product Natural Gradient Method for Deep Learning

In this paper, a novel second-order method called NG+ is proposed. By following the rule "the shape of the gradient equals the shape of the parameter", we define a generalized fisher information matrix (GFIM) using the products of gradients in the matrix form rather than the traditional vectorization. Then, our generalized natural gradient direction is simply the inverse of the GFIM multiplies the gradient in the matrix form. Moreover, the GFIM and its inverse keeps the same for multiple steps so that the computational cost can be controlled and is comparable with the first-order methods. A global convergence is established under some mild conditions and a regret bound is also given for the online learning setting. Numerical results on image classification with ResNet50, quantum chemistry modeling with Schnet, neural machine translation with Transformer and recommendation system with DLRM illustrate that GN+ is competitive with the state-of-the-art methods.

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MS12

On the Surprising (but Fragile) Optimality of Affine Decision Rules

Affine decision rules are a popular solution method for two stage distributionally robust optimization problems, resulting in highly tractable optimization problems. However, their simple structure implies that affine decision rules can result in crude approximations. In this study, we provide necessary conditions for the structure of a two stage distributionally robust problem to afford affine decision rules that correspond to optimal decisions. Unlike related results from the literature that focus on two-stage robust problems, our results hold for the distributionally robust setting that encompasses two-stage robust and stochastic programs as special cases. We demonstrate our results on several applications of practical interest.

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MS12

From Affine to Threshold Policies: A New Framework in Dynamic Robust Optimization

Affine policies are widely used as a solution approach in dynamic optimization where computing an optimal adjustable solution is usually intractable. While the worst case performance of affine policies can be significantly bad, the empirical performance is observed to be near-optimal for a large class of problem instances. For instance, in the two-stage dynamic robust optimization problem with linear covering constraints and uncertain right hand side, the worst-case approximation bound for affine policies is O(vm) that is also tight whereas observed empirical performance is near-optimal. This work aims to address this stark-contrast between the worst-case and the empirical performance of affine policies and use those insights to efficiently construct near-optimal threshold policies.

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MS12

Improved Decision Rule Approximations for Multi-Stage Robust Optimization via Copositive Programming

We study decision rule approximations for generic multi-stage robust linear optimization problems. We consider linear decision rules for the case when the objective coefficients, the recourse matrices, and the right-hand sides are uncertain, and consider quadratic decision rules for the case when only the right-hand sides are uncertain. The resulting optimization problems are NP-hard but amenable to copositive programming reformulations that give rise to tight conservative approximations. We further enhance these approximations through new piecewise decision rule schemes. Finally, we prove that our proposed approximations are tighter than the state-of-the-art schemes and demonstrate their superiority through numerical experiments.

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MS12

Robustness Optimization

We present a model for optimization under uncertainty called robustness optimization that favors solutions for which the models constraint would be the most robust or least fragile under uncertainty. The decision maker does not have to size the uncertainty set, but specifies an acceptable target, or loss of optimality compared to the baseline model, as a tradeoff for the models ability to withstand greater uncertainty. We axiomatize the decision criterion associated with robustness optimization, termed as the fragility measure, which is a class of Brown and Sim (2009) satisficing measure, and it satisfies the properties of monotonicity, positive homogeneity, subadditivity, pro-robustness, and anti-fragility. We provide a representation theorem and connect it with known fragility measures including the decision criterion associated with the GRC-sum of Ben-Tal et al. (2017) and the riskiness index of Aumann and Serrano (2008). We present a suite of practicable robustness optimization models for prescriptive analytics including linear, adaptive linear, data- driven adaptive linear, combinatorial and dynamic optimization problems.

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MS13

Symmetry Reduction for Conic Optimization over the Doubly Nonnegative Cone

A common computational approach for combinatorial optimization problems is to use (hierarchies of) semidefinite programming (SDP) relaxations. These SDP problems typically involve nonnegative matrices, i.e. they are conic optimization problems over the doubly nonnegative cone. The Jordan reduction, a symmetry reduction method for conic optimization, was recently introduced for symmetric cones by Parrilo and Permenter [Mathematical Programming 181(1), 2020]. We extend this method to the doubly nonnegative cone, and investigate its application to known relaxations of the quadratic assignment and maximum stable set problems. We also introduce new Julia software where the symmetry reduction is implemented. This is joint work with Daniel Brosch.

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MS13

Computing the Nearest Doubly Stochastic Matrix by a Newton-Type Method

In this talk, we present a Newton-type method for finding the nearest doubly stochastic matrix in the Frobenius norm to a given matrix. The optimality condition of this problem can be stated as a system of strongly semismooth functions. We study a Newton-type method to solve this system, and thus finding the nearest doubly stochastic matrix. We provide a sufficient condition for the quadratic convergence of the semismooth Newton method. We also propose a modified Newton method for the general case. This is a joint work with Haesol Im, Xinxin Li and Henry Wolkowicz.

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MS13

Symmetry Reduction to Optimize a Hypergraph-Based Polynomial from Queuing Theory

Given integers $n, d \geq 2$, let $([n], E)$ denote the complete graph on n elements, and consider the following homogeneous multivariate polynomial in variables $x = (x_e : e \in E)$:

$$f_d(x) = \sum_{(e_1,\ldots,e_d)\in E^d} \prod_{i=1}^{d} \frac{x_{e_i}}{|e_1 \cup \ldots \cup e_i|}.$$

Cardinaels, Borst, van Leeuwaarden [arXiv:2005.14566, 2020] asked whether f_d (which arises in a model of job-occupancy in redundancy scheduling) attains its minimum over the standard simplex at the uniform probability vector. Brosch, Laurent and Steenkamp [arXiv:2009.04510, 2020] showed that f_d is convex if $d = 2$ and $d = 3$, implying the desired result for these d. We use representation theory to prove the following. Fix an integer k. For each $n \geq k$, let S_{n-k} act on $[n]$ by permuting $\{k+1, \ldots, n\}$. Suppose that

$$A^{(n)} \in \mathbb{R}^{\binom{[n]}{2} \times \binom{[n]}{2}}$$

for each $n \geq k$ are symmetric matrices such that each $A^{(n)}$ is invariant under the simultaneous action of S_{n-k} on its rows and columns and such that for all $n, n' \in \mathbb{N}$ with $k \leq n' \leq n$ and all $e_i, e_j \in \binom{[n']}{2}$, we have $A^{(n')}_{e_i,e_j} = A^{(n)}_{e_i,e_j}$. Then $A^{(n)}$ is positive semidefinite for every $n \geq k$ if and only if three constant matrices (with order and coefficients independent of n) are positive semidefinite. This result is then used in combination with a computer-assisted verification to show that f_d is convex for $d \leq 8$.

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MS13

SDP-Based Bounds for Graph Partitioning Problems by Extended ADMM

This talk will discuss two NP-hard graph partitioning problems, k-equipartitioning problems, and graph partitioning with knapsack constraints (GPKC). We will show the tight SDP relaxations with nonnegativity constraints for those two problems and how to get the lower bounds via extended alternating direction methods with multipliers (ADMM) to efficiently solve those large-scale SDP problems. We will also introduce the heuristics used to generate the upper bounds for the original problems from the SDP solutions with little cheap computational expense.

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MS14

On the Treatment of Optimization Problems with

L1 Penalty Terms via Multiobjective Continuation

In many areas it is of great importance to find sparse models, especially in image and signal processing, machine learning and medical imaging. One of the motivations is to ensure robustness against noisy data, but also to find models that are as simple as possible and therefore easier to interpret. It is common practice to assess the sparsity using the l^1-norm and to solve the problem using a regularization parameter, i.e. $f(x) + \lambda\|x\|_1$ with $\lambda \in (0,1)$ is solved. In order to gain a better understanding and to allow for an informed model selection, we will not use this weighted-sum approach. Instead, we aim at solving the corresponding multiobjective optimization problem, i.e.

$$\min_{x\in\mathbb{R}^n} \begin{pmatrix} f(x) \\ \|x\|_1 \end{pmatrix}.$$

We will present a Continuation Method, which is specifically tailored to the l^1-norm as a second objective function and discuss the advantages but also future challenges of our method in practice.

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MS14

Interactive Multiobjective Evolutionary Optimization using Multiple Achievement Scalarizing Functions: Extending a New Paradigm

The objectives of multiobjective optimization problems (MOPs) are typically conflicting in nature. Accordingly, instead of having a single optimal solution, MOPs have a set of optimal solutions with different trade-offs forming a Pareto front in the objective space. Evolutionary algorithms (EAs) have been used in the literature to solve MOPs. However, applying EAs is inefficient with an increasing number of objectives. Another way to solve MOPs is to use scalarizing functions (SFs). They use preferences of a decision maker (DM) to convert a MOP into a scalar valued optimization problem, which can be solved using e.g., mathematical optimization methods to get one Pareto optimal solution at a time. However, the DM may wish to see more than one solution at a time to learn more about the problem. We have recently proposed a new paradigm for solving MOPs by creating a new space, called a Preference Incorporated Space (PIS). The novel IOPIS algorithm replaces original objectives by a small number of SFs to interactively create the PIS and uses EAs to optimize them. Using IOPIS yields diverse solutions that still follow the preference of the DM. In this paper, we extend the IOPIS algorithm from two to a diverse set of SFs using the parameterized GLIDE formulation that enables using multiple types of preference information. We study the effect of using different combinations of SFs on solution quality and efficiency. This research is a part of the open-source Python framework DESDEO.

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MS14

Pareto Explorer: a Global/Local Exploration Tool for Many-Objective Optimization Problems

Optimization problems where several objectives have to be considered concurrently arise naturally in many applications. Since decision making processes are getting more and more complex, there is a recent trend to consider more and more objectives in such problems, known and many objective optimization problems (MaOPs). For such problems it is not possible any more to compute finite size approximations of the entire solution set. In this presentation, we will present the Pareto Explorer (PE) for the numerical treatment of MaOPs. The PE is a global/local exploration tool that consists of two steps: first, an optimal solution of the given MaOP is selected via a global solver. In a next step, the Pareto landscape around this point is explored around this solution according to the users preferences that can be articulated in decision variable, objective, or weight space. We finally demonstrate the effectiveness of the PE on several MaOPs related to real-world problems.

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MS14

Numerical Differentiation of Noisy Data: A Unifying Multi-Objective Optimization Framework

Computing derivatives of noisy measurement data is ubiquitous in the physical, engineering, and biological sciences, and it is often a critical step in developing dynamic models or designing control. Unfortunately, the mathematical formulation of numerical differentiation is typically ill-posed, and researchers often resort to an ad hoc process for choosing one of many computational methods and its parameters. In this work, we take a principled approach and propose a multi-objective optimization framework for choosing parameters that minimize a loss function to balance the faithfulness and smoothness of the derivative estimate. Our framework has three significant advantages. First, the task of selecting multiple parameters is reduced to choosing a single hyper-parameter. Second, where ground-truth data is unknown, we provide a heuristic for selecting this hyper-parameter based on the power spectrum and temporal resolution of the data. Third, the optimal value of the hyper-parameter is consistent across different differentiation methods, thus our approach unifies vastly different numerical differentiation methods and facilitates unbiased comparison of their results. Finally, we provide an extensive open-source Python library pynumdiff to facilitate easy application to diverse datasets: https://github.com/florisvb/PyNumDiff.

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MS15

A Bilevel Learning Approach for Optimal Observation Placement in Variational Data Assimilation

In this work, we propose a bilevel optimization approach for the placement of space and time observations in variational data assimilation problems. Within the framework of supervised learning, we consider a bilevel problem where the lower-level task is the variational reconstruction of the initial condition of a semilinear system, and the upper-level problem solves the optimal placement with the help of a sparsity inducing function. Due to the pointwise nature of the observations, an optimality system with regular Borel measures is obtained as necessary optimality condition for the lower-level problem. The latter is then considered as constraint for the upper-level instance, yielding an optimization problem constrained by a multi-state system with measures. We demonstrate Lagrange multipliers' existence and derive a necessary optimality system characterizing the optimal solutions of the bilevel problem. The numerical solution is carried out also on two levels. The lower-level problem is solved using a standard BFGS method, while the upper-level one is solved using a projected BFGS algorithm, based on the estimation of ϵ-active sets. Finally, some numerical experiments are presented to illustrate the main features of our approach.

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MS15

Implicit Variables in Hierarchical Programming

Many practically relevant classes of optimization problems comprise so-called implicit variables which are, as the name suggests, implicitly used to model feasibility conditions but do not appear in the objective function. Often such variables are treated as explicit ones in order to tackle the underlying optimization problem via available tools from optimization theory. As we will show, this approach has several drawbacks comprising the generation of artificial local minimizers as well as the need for stronger constraint qualifications in the reformulated problem. We discuss these issues by means of the fairly general model problem

$$\min_z \left\{ f(z) \,|\, 0 \in \bigcup\nolimits_{\lambda \in F(z)} G(z,\lambda),\, z \in M \right\}$$

where $f\colon \mathbb{R}^n \to \mathbb{R}$ is locally Lipschitzian, $F\colon \mathbb{R}^n \rightrightarrows \mathbb{R}^m$ as well as $G\colon \mathbb{R}^n \times \mathbb{R}^m \rightrightarrows \mathbb{R}^\ell$ are set-valued mappings possessing closed graphs, respectively, and $M \subset \mathbb{R}^n$ is a closed set. Here, λ plays the role of an implicit variable. We discuss our findings in the context of hierarchical optimization. More precisely, we tackle bilevel optimization problems and evaluated multiobjective optimization problems with the obtained theory.

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MS15

Automatic Distributed Regularization Parameter Selection in Total Generalized Variation Based Image Reconstruction via Bilevel Optimization

Total Generalized Variation (TGV) is an established high quality regularizer for a variety of variational image reconstruction tasks. By incorporating an infimal convolution type combination of first and second order derivatives in the regularization process it avoids the staircasing effect of Total Variation (TV), while preserving the image edges. The regularization effect of TGV is dictated by two regularization parameters, whose determination remains a challenging task. In this work we apply a bilevel optimization framework with a suitable statistics-based upper level objective, in order to automatically select these parameters. The framework allows for the parameters to be spatially distributed, thus better recovering high-detailed areas in the image. Denoising tests confirm that the automatically selected distributed regularization parameters lead in general to an improved reconstruction quality.

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MS15

Optimal Selection of the Spatially Variant Differential Order in a Fractional Laplacian Model

In this talk, we focus on a fractional model with spatially variant differential order and the optimal selection thereof. Concerning the model: we provide a formulation in function space, analyze existence and stability of solutions, and further provide a solution algorithm together with numerical tests. Further, we establish parameter selection procedures using noise statistics and edge detection that can be embedded in a bilevel optimization problem. The analysis of the problem requires the use of non-Muckenhoupt weighted Sobolev spaces and non-standard trace results. We finalize the talk with possible future research directions and open problems.

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MS16

Distributed Policy Gradient Approach for Multi-Agent Multi-Task Reinforcement Learning

We develop a mathematical framework for solving multi-task reinforcement learning (MTRL) problems based on a type of decentralized policy gradient method. The goal in MTRL is to learn a common policy that operates effectively in different environments; these environments have similar (or overlapping) state and action spaces, but have different rewards and dynamics. Agents immersed in each of these environments communicate with other agents by sharing their models (i.e. their policy parameterizations) but not their state/reward paths. Our analysis provides a convergence rate for a consensus-based distributed policy gradient method for finding such a policy. We demonstrate the effectiveness of the proposed method using a series of numerical experiments. These experiments range from small-scale "Grid World" problems that readily demonstrate the trade-offs involved in multi-task learning to large-scale problems, where common policies are learned to play multiple Atari games or to navigate an airborne drone in multiple (simulated) environments.

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MS16

The Role of Coordination in Distributed Accelerated Optimization over Networks

We present a new class of accelerated distributed algorithms for the robust solution of convex optimization problems over networks. The novelty of the approach lies in the introduction of distributed restarting mechanisms that coordinate the evolution of accelerated optimization dynamics with individual asynchronous and periodic time-varying momentum coefficients. We model the algorithms as set-valued hybrid dynamical systems since the method combines continuous-time dynamics with acceleration and set-valued discrete-time restarting updates. For these dynamics, we derive graph-dependent restarting conditions that guarantee suitable stability, robustness, and convergence properties in distributed optimization problems characterized by strongly convex primal functions. Our results are illustrated via numerical examples.

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MS16

Parameter Estimation in Epidemic Spread Networks using Limited Measurements

We study the problem of estimating the parameters (i.e., infection rate and recovery rate) governing the spread of epidemics in networks. Such parameters are typically estimated by measuring various characteristics (such as the number of infected and recovered individuals) of the infected populations over time. However, these measurements also incur certain costs, depending on the population being tested and the times at which the tests are administered. We thus formulate the epidemic parameter estimation problem as an optimization problem, where the goal is to either minimize the total cost spent on collecting measurements, or to optimize the parameter estimates while remaining within a measurement budget. We show that these problems are NP-hard to solve in general, and then propose approximation algorithms with performance guarantees. We validate our algorithms using numerical examples.

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MS16

Finite-Time Guarantees for Byzantine-Resilient Distributed State Estimation with Noisy Measurements

This work considers resilient, cooperative state estimation in unreliable multi-agent networks. A network of agents aims to collaboratively estimate the value of an unknown vector parameter, while an *unknown* subset of agents suffer Byzantine faults. Faulty agents malfunction arbitrarily and may send out *highly unstructured* messages to other agents in the network. As opposed to fault-free networks, reaching agreement in the presence of Byzantine faults is far from trivial. In this paper, we propose a computationally-efficient algorithm that is provably robust to Byzantine faults. At each iteration of the algorithm, a good agent (1) performs a gradient descent update based on noisy local measurements, (2) exchanges its update with other agents in its neighborhood, and (3) robustly aggregates the received messages using coordinate-wise trimmed means. Under mild technical assumptions, we establish that good agents learn the true parameter asymptotically in almost sure sense. We further complement our analysis by proving (high probability) *finite-time* convergence rate.

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MS17

Structure in Min-Max Optimization (and How to

Use It)

Min-max optimization problems have received significant recent renewed interest, due to their applications in machine learning, and in particular in empirical risk minimization (ERM) and adversarial training. Although deceptively similar to standard optimization, min-max optimization has unique features that often lead natural approaches such as gradient descent-type updates to fail even on relatively mild problem instances. Further, the types of guarantees that can be established are generally more restricted than in the counterpart setups of standard convex or smooth nonconvex optimization. I will discuss how introducing structure into the min-max optimization problems can be used to surpass many of the obstacles raised by the worst-case instances. First is a novel Lipschitz condition for the gradients that is natural in many ERM problems and leads to a fast cyclic coordinate method that significantly improves upon existing results even in the standard convex case. Second is the separable structure of ERM problems that can be utilized to obtain faster variance-reduced methods, even surpassing the obstacles of existing lower bounds for general composite optimization. Finally, I will discuss a novel structural condition for nonconvex-nonconcave setups that is present in many problem instances and allows guaranteeing convergence of an Extragradient-type method, surpassing the impossibility results that exist for general smooth nonconvex-nonconcave min-max optimization.

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MS17

Faster First-Order Primal-Dual Methods for Linear Programming using Restarts and Sharpness

Restart schemes have been used to improve the convergence on several algorithms including accelerated gradient descent and subgradient descent. In this work, we study restart schemes for primal-dual first-order methods such as primal-dual hybrid gradient, extragradient, and ADMM. We show that these methods with a fixed frequency or adaptive restart scheme achieve linear convergence when they are applied to linear programs. For primal-dual hybrid gradient our restart schemes achieves the optimal convergence rate and that without restarts the method is suboptimal. Experiments with primal-dual hybrid gradient show our adaptive restart scheme dramatically improves the ability of the method to obtain high accuracy solutions.

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MS17

An $O(s^r)$-Resolution Ode Framework for Understanding Discrete-Time Algorithms and Applications to the Linear Convergence of Minimax Problems

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MS18

On Solving Large-Scale Nonconvex Stochastic Programming Problems using High-Performance Computing

Exploiting problem structure is quintessential in improving the state-of-the-art in optimization algorithms and in enabling the efficient use of high-performance, massively parallel computing platforms. Motivated by concrete applications in the optimization of the electrical power grid and structural design optimization, the presentation covers optimization algorithms of quasi-Newton flavor for nonlinear continuous optimization problems of extreme sizes. The focus is on addressing computational challenges at scale by exploiting problems structures to improve on the algorithm complexity and to expose decomposition opportunities suitable for massively parallel computing. Computational results obtained on a couple of high-performance computing (HPC) platforms, which include the Summit supercomputer, will be also presented and discussed in the light of the underlying optimization problems, namely, security constrained optimal power flow and compliance topology optimization.

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MS18

ALESQP: An Augmented Lagrangian Equality-Constrained SQP Method for Optimization with General Constraints

We present a new algorithm for infinite-dimensional optimization with general constraints, called ALESQP. In a nutshell, ALESQP is an augmented Lagrangian method that penalizes inequality constraints and solves equality-constrained nonlinear optimization subproblems at every iteration. The subproblems are solved using a matrix-free trust-region sequential quadratic programming (SQP) method that takes advantage of inexact linear solvers. Another key feature of ALESQP is a constraint decomposition strategy that allows it to exploit problem-specific variable scalings and inner products. We analyze convergence of ALESQP under different assumptions. We show that strong accumulation points are stationary, i.e., in finite dimensions ALESQP converges to a stationary point. In infinite dimensions we establish that weak accumulation points are feasible in many practical situations. Under additional assumptions we show that weak accumulation points are stationary. We present examples from optimal control, where ALESQP shows remarkable discretization-independent performance, requiring a modest number of iterations to meet constraint tolerances at the level of machine precision. Also, we demonstrate a fully matrix-free solution of an infinite-dimensional problem with nonlinear inequality constraints, with scalable performance in all iterative components of ALESQP, including the augmented-Lagrangian iteration, the SQP subproblem solver and SQP's quadratic optimization solver.

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MS18

A Primal Dual Projection Algorithm for Efficient Constraint Preconditioning

We consider a linear iterative solver for large scale linearly constrained quadratic minimization problems that arise, for example, in optimization with partial differential equations (PDEs). By a primal-dual projection (PDP) iteration, which can be interpreted and analysed as a gradient method on a quotient space, the given problem can be solved by computing sulutions for a sequence of constrained surrogate problems, projections onto the feasible subspaces, and Lagrange multiplier updates. As a major application we consider a class of optimization problems with PDEs, where PDP can be applied together with a projected cg method using a block triangular constraint preconditioner. Numerical experiments show reliable and competitive performance for an optimal control problem in elasticity.

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MS18

Overlapping Schwarz Algorithms for Graph-Structured Nonlinear Programs

In this work, we present an overlapping Schwarz framework for solving graph-structured optimization problems. The proposed approach is implemented in the Julia-based nonlinear programming solver (that we call MadNLP.jl) that is interfaced to the graph-based modeling package Plasmo.jl. The efficiency of this framework is demonstrated via problems arising in transient gas network optimization and multi-period AC optimal power flow.

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MS19

Surrogate Modeling of Simulations for Multiobjective Optimization Applications

Many real-world blackbox multiobjective optimization problems are derived from complex numerical simulations. However, the objectives may not be the direct result of simulations, but rather algebraic functions of simulation outputs. As an example, consider the case where numerous simulation outputs are being minimized, and they are condensed into a smaller number of objectives by applying algebraic utility functions (e.g., sum-of-squares). One could consider each objective as an individual blackbox function. However, this approach would require each contributing simulation to be evaluated each time that a utility function is evaluated. Furthermore, this approach would lose precious information about the structure of the utility functions. In this talk, we consider the advantages (both computational and theoretical) of considering simulations separately from objectives, specifically, in the context of surrogate modeling.

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MS19

Using First-Order Information in Direct Multi-Search

Derivatives are an important tool for single-objective optimization. In fact, it is commonly accepted that derivative-based methods present a better performance than derivative-free optimization approaches. In this work, we will start by showing that the same does not apply to multiobjective derivative-based optimization, when the goal is to compute an approximation to the complete Pareto front of a given problem. The competitiveness of Direct MultiSearch (DMS), a robust and efficient derivative-free optimization algorithm, will be stated for derivative-based multiobjective optimization problems. Derivatives will then be used to prune the positive spanning sets considered at the poll step of the algorithm, highlighting the role that ascent directions, that conform to the geometry of the nearby feasible region, can have when computing approximations to the entire Pareto front of a given multiobjective optimization problem. This new variant of DMS, which prunes the poll set of directions, but that at some iterations considers its enrichment with ascent directions, shows to be competitive not only with derivative-based solvers but also with the original implementation of DMS.

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MS19

On the Hausdorff Distance between a Pareto Set and its Discretization

Unlike deterministic multi-objective optimization algorithms, which usually return only decision vectors whose images do not dominate each other, multi-objective simulation optimization algorithms may return a set of decision vectors containing at least one point whose image dominates another when both are evaluated without error. Thus, error bounds and metrics for evaluating multi-objective simulation optimization algorithms should account for the possibility that these extra points are included in the returned set. Toward this end, we discuss the Hausdorff distance between a Pareto set and its discretization; we also discuss the relevance of our results to multi-objective simulation optimization.

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MS19

Achieving Well-Distributed Points on the Pareto Front for p¿2 dimensions

Engineers designing a system require a complete picture of the possible tradeoffs. Mathematically, this means a good description of the Pareto front. For $p > 2$ objectives finding a well-distributed set of points on the Pareto front (as measured by statistical discrepancy) is challenging. If the computed point set has high discrepancy, the cost of additional Pareto points to fill out the tradeoff picture may be prohibitive. A polynomial complexity scheme to produce a low discrepancy Pareto point set based on Delaunay triangles is proposed, and implemented in VTMOP.

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MS20

Dealing with Constraints in Distributed Optimization over Networks

This talk deals with distributed convex optimization subjected to constraints. To be able to tackle large scale problems we present their penalty reformulations. We discuss the choice of penalty functions as well as time-varying penalty parameters which would guarantee convergence to a solution given directed time-varying communication graphs. Moreover, for a specific class of problems we estimate the convergence rate for the proposed penalty-based gradient method.

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MS20

A Distributed Cubic-Regularized Newton Method for Smooth Convex Optimization over Networks

We propose a distributed, cubic-regularized Newton method for large-scale convex optimization over networks. The proposed method requires only local computations and communications and is suitable for federated learning applications over arbitrary network topologies. We show a $O(k^{-3})$ convergence rate when the cost function is convex with Lipschitz gradient and Hessian, with k being the number of iterations. We further provide network-dependent bounds for the communication required in each step of the algorithm. We provide numerical experiments that validate our theoretical results.

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MS20

On the Convergence of Consensus Algorithms with Markovian Noise and Gradient Bias

This paper presents a finite time convergence analysis for a decentralized stochastic approximation (SA) scheme. The scheme generalizes several algorithms for decentralized machine learning and multi-agent reinforcement learning. Our proof technique involves separating the iterates into their respective consensual parts and consensus error. The consensus error is bounded in terms of the stationarity of the consensual part, while the updates of the consensual part can be analyzed as a perturbed SA scheme. Under the Markovian noise and time varying communication graph assumptions, the decentralized SA scheme has an expected convergence rate of $O(\log T/\sqrt{T})$, where T is the iteration number, in terms of squared norms of gradient for nonlinear SA with smooth but non-convex cost function. This rate is comparable to the best known performances of SA in a centralized setting with a non-convex potential function.

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MS20

Distributed Optimization for Problems with Variational Inequality Constraints

Traditionally, the mathematical models and algorithms for constrained distributed optimization over networks have been much focused on the cases where the functional constraints are in the form of inequalities, equalities, or easy-to-project sets. In the first part of this talk, we consider a class of optimization problems with variational inequality constraints. This mathematical formulation captures a wide range of models including those complicated by the presence of equilibrium constraints, complementarity constraints, or an inner-level large scale optimization problem. To address the proposed model, we develop randomized and distributed first-order methods equipped with new non-asymptotic convergence rates. In the second part of the talk, we consider a special case of the proposed model that is characterized as a bilevel distributed optimization model. Employing a novel regularization-based relaxation approach and the recently emerged gradient-tracking techniques, we develop an iteratively regularized push-pull gradient algorithm. We establish the consensus and derive new convergence rate statements for suboptimality and infeasibility of the generated iterates for solving the bilevel model. The numerical performance of the proposed algorithms is presented in different examples in game theory, image processing, and machine learning.

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MS21

The Strip Method for Shape Derivatives

A major challenge in shape optimization is the coupling of finite element method (FEM) codes in a way that facilitates efficient computation of shape derivatives. This is particularly difficult with multiphysics problems involving legacy codes, where the costs of implementing and maintaining shape derivative capabilities are prohibitive. The volume and boundary methods are two approaches to computing shape derivatives. Each has a major drawback: the boundary method is less accurate, while the volume method is more invasive to the FEM code. We introduce the strip method, which computes shape derivatives on a strip adjacent to the boundary. The strip method makes code coupling simple. Like the boundary method, it queries the state and adjoint solutions at quadrature nodes, but requires no knowledge of the FEM code implementations. At the same time, it exhibits the higher accuracy of the volume method. As an added benefit, its computational complexity is comparable to that of the boundary method, i.e., it is faster than the volume method. We illustrate the benefits of the strip method with numerical examples.

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MS21

Shape and Geometry Analysis in Images using Scikit-Shape

Many problems in science and engineering are expressed as shape optimization problems, in which the variable is a shape such as a set of 2d curves. Examples are optimization of the shape of an airplane wing, and delineation of boundaries of biological structures in medical scans. We typically express such problems as energies with data (or target) mismatch and geometric regularization components, to be minimized algorithmically to attain the optimal shape. To solve such problems, we have implemented a suite comprising various building blocks of such problems and algorithms to perform the minimization, including geometric regularization, statistical shape priors, adaptive geometric discretization, and fast Newton-type minimization schemes. Moreover, we have developed crucial shape analysis algorithms for statistical analysis and evaluation of the shapes computed, based on elastic shape distance framework. Our main applications are image and data analysis problems, but the infrastructure is quite general, and can be used for problems in other fields as well. All our algorithms are implemented in Python, leveraging on the NumPy/SciPy ecosystem, making them as easy to use as Matlab, also compatible with existing Python tools. Our algorithms will be freely available as an open source package for the research community at: http://scikit-shape.org

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MS21

A Continuous Perspective on Shape Optimization

We consider shape optimization problems as optimal control problems via the method of mappings. Instead of optimizing over a set of admissible shapes a reference domain is introduced, and it is optimized over a set of admissible transformations. The focus is on the choice of the set of admissible transformations, which we motivate from a continuous perspective. In order to guarantee local injectivity of the admissible transformations we enrich the optimization problem by a nonlinear constraint. Moreover, we work with scalar valued functions on the design boundary and extension equations to define the set of admissible transformations. Choices of the extension equation are discussed and numerical results are presented.

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MS21

Constrained Shape Optimization in Shape Spaces: From Deterministic to Stochastic Models

A challenge in shape optimization is in the modeling of shapes, which do not inherently have a vector space structure. If one cannot work in vector spaces, one possible approach is to cast the sets of shapes in a Riemannian viewpoint, where each shape is a point on an abstract space like a manifoldor, more generally, a diffeological spaceequipped with a notion of distances between shapes. In this talk, we first apply the differential-geometric structure of Riemannian shape spaces to the theory of deterministic shape optimization problems. Since many relevant problems in the area of shape optimization involve a constraint in the form of a partial differential equation, which contains inputs or material properties that may be unknown or subject to uncertainty, we consider also stochastic shape optimization problems. We present a novel method, which is the extension of the classical stochastic gradient method to infinite-dimensional shape manifolds. The method is demonstrated on a shape optimization problem. A motivation for our model is in electrical impedance tomography, where the material distribution of electrical properties such as electric conductivity and permittivity inside the body is to be determined.

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MS22

Parameter Learning in Alternating Direction Method of Multipliers

For many large-scale physical networked systems, like sensor networks, autonomous vehicle fleets, and electric power systems, optimization and control tasks are traditionally performed using centralized methods. However, centralized methods pose scalability issues as network size and complexity increase, which limits computational tractability. Many researchers have instead proposed the use of distributed methods, which spread computation across the network and enable parallelization and, hence, superior scalability. Yet, there still exist major barriers to the implementation of distributed methods, most notably, ensuring fast convergence. Common distributed methods like ADMM (Alternating Direction Method of Multipliers) can take many iterations to converge to a sufficiently high accuracy and have convergence guarantees only for a limited class of problems. Furthermore, the convergence rate is strongly correlated with the choice of penalty or stepsize parameters, which are traditionally defined heuristically at each iteration. To address these challenges, we develop a policy that learns the parameter values iteration-to-iteration that accelerate the convergence rate. Specifically, we use constrained reinforcement learning techniques to select parameters and train our policy using advanced neural network models. We demonstrate this parameter learning method for component-based ADMM within the context of electric power systems via the distributed AC Optimal Power Flow problem.

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MS22

Distributed Optimal Power Flow Algorithms with Nonideal Communications

To address rapidly growing quantities of distributed energy resources (e.g., solar PV generators, battery storage systems, responsive demands), power system operators are considering the adoption of distributed optimization algorithms that leverage communications among various agents to determine minimum-cost operating points. Computing these operating points by solving optimal power flow problems in a distributed fashion has potential advantages in scalability, flexibility, privacy, and robustness. Data quality plays a major rule in the performance of distributed algorithms. This presentation describes the impacts of data quality on the performance of three distributed optimization algorithms (Alternating Direction Method of Multipliers, Analytic Target Cascading, and Auxiliary Principal Problem) when applied to optimal power flow problems. We compare the performance of these algorithms in terms of their convergence rates and solution accuracy under three data quality models: (1) additive Gaussian noise, (2) bad data, and (3) intermittent communication failure. This presentation also discusses the cybersecurity implications of the existence of compromised agents that do not faithfully execute the distributed optimization algorithm.

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MS22

A Privacy-Preserving Distributed Control of Optimal Power Flow

We consider a distributed optimal power flow formulated as an optimization problem that maximizes a nondifferentiable concave function. Solving such a problem by the existing distributed algorithms can lead to data privacy issues because the solution information exchanged within the algorithms can be utilized by an adversary to infer the data. To preserve data privacy, in this paper we propose a differentially private projected subgradient (DP-PS) algorithm that includes a solution encryption step. We show that a sequence generated by DP-PS converges in expectation, in probability, and with probability 1. Moreover, we show that the rate of convergence in expectation is affected by a target privacy level of DP-PS chosen by the user. We conduct numerical experiments that demonstrate the convergence and data privacy preservation of DP-PS.

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MS22

A Two-Level ADMM Algorithm for AC OPF with Convergence Guarantees

In this talk, we propose a two-level distributed algorithmic framework for solving the AC optimal power flow (OPF) problem with convergence guarantees. The presence of highly nonconvex constraints in OPF poses significant challenges to distributed algorithms based on the alternating direction method of multipliers (ADMM). In particular, convergence is not provably guaranteed for nonconvex network optimization problems like AC OPF. In order to overcome this difficulty, we propose a new distributed reformulation for AC OPF and a two-level ADMM algorithm that goes beyond the standard framework of ADMM. We will establish the global convergence and iteration complexity of the proposed algorithm under mild assumptions. Extensive numerical experiments over some largest test cases from NESTA and PGLib-OPF (up to 30,000-bus systems) demonstrate advantages of the proposed algorithm over existing ADMM variants in terms of convergence, scalability, and robustness. Moreover, under appropriate parallel implementation, the proposed algorithm exhibits fast convergence comparable to or even better than the state-of-the-art centralized solver.

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MS23

Self-Supervised Deep Learning for Individualized Brain Functional Network Identification

Intrinsic functional connectivity magnetic resonance imaging (fcMRI) is a powerful tool to study the organization of functional networks (FNs) in the human brain. Recent work based on advances in image analytics has established that FNs are in fact person-specific. However, the translational promise of person-specific FNs is at present hindered by several obstacles. In particular, to enforce correspondence across different subjects personalized FNs are typically computed under certain constraints, which may yield biased results. To address this limitation, we develop a novel self-supervised deep learning method to identify person-specific FNs in an end-to-end learning fashion. Our method leverages deep Encoder-Decoder networks and conventional functional brain decomposition models to identify person-specific FNs in a self-supervised learning framework by optimizing data fitting and sparsity regularization terms that are commonly used in functional brain decomposition models. The proposed method has been validated based on multiple fcMRI datasets and experimental results have demonstrated that our method could obtain person-specific FNs which are consistent with well-established FNs and are informative for predicting brain age, indicating that the person-specific FNs identified truly captured the underlying variability of individualized functional neuroanatomy.

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MS23

Joint Optimization of Learning-Based Image Reconstruction and Sampling for MRI

Machine learning approaches to medical image reconstruction are of considerable recent interest, especially supervised approaches that use a corpus of training data. Accelerated MRI scans, where fewer k-space points than image voxels are acquired, is a natural setting for such reconstruction methods. Recently, machine learning methods for optimizing the k-space sampling have also had growing interest. This talk will summarize recent work where we jointly optimize non-Cartesian k-space sampling, heeding physical constraints like gradient slew rate, and a learning-based image reconstruction method that originates from a large-scale optimization approach.

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MS23

Statistical Estimation of Mass Effect using Ensemble Image-Registration

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MS24

A Matrix Positivstellensatz with Lifting Polynomials

Given the projections of two semialgebraic sets defined by polynomial matrix inequalities, we talk about how to determine whether one is contained in the other. To address this issue, a new matrix Positivstellensatz with lifting polynomials is proposed. Under some general assumptions (e.g., the archimedeanness, nonempty interior, convexity), we prove that such a containment holds if and only if the proposed matrix Positivstellensatz is satisfied. The corresponding certificate can be searched for by solving a semidefinite program. An important application is to certify when a spectrahedrop (i.e., the projection of a spectrahedron) is contained in another one.

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MS24

Amenable Cones are Particularly Nice

Amenability is a geometric property of convex cones that is stronger than facial exposedness and assists in the study of error bounds for conic feasibility problems. In this talk I will focus on the relationships between amenability and other properties of convex cones, such as niceness and projectional exposure, and will also mention several open questions that we werent able to resolve. The talk is based on a joint work with Bruno Loureno and James Saunderson, https://arxiv.org/abs/2011.07745.

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MS24

On Computing Nonlinearity Intervals in Parametric Semidefinite Optimization

We introduce the notions of nonlinearity interval and transition point of the optimal partition for a parametric semidefinite optimization problem. We provide conditions for the existence of a nonlinearity interval and show that the continuity of the optimal set mapping might fail on a nonlinearity interval. Furthermore, under a nonsingularity assumption, we prove that the set of singular points and the set of points at which the optimal set mapping is discontinuous are finite. We then present a methodology, stemming from numerical algebraic geometry, to efficiently compute nonlinearity intervals and transition points of the optimal partition.

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MS24

How to Construct any Weakly Infeasible Semidefinite Program and Bad Projection of the PSD Cone?

A weakly infeasible semidefinite program (SDP) has no feasible solution, but it has nearly feasible solutions that approximate the constraint set to arbitrary precision. These SDPs are ill-posed and numerically often unsolvable. They are also closely related to "bad" linear projections that map the cone of positive semidefinite matrices to a nonclosed set. We describe a simple echelon form of weakly infeasible SDPs with the following properties: it is obtained by elementary row operations and congruence transformations; it makes weak infeasibility evident; and using it we can construct any weakly infeasible SDP or bad linear projection by an elementary combinatorial algorithm. We also prove that some SDPs in the literature are in our echelon form, for example, the SDP from the sum-of-squares relaxation of minimizing the famous Motzkin polynomial.

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MS26

Sparsity, Feature Selection and the Shapley Folkman Theorem

The Shapley Folkman theorem acts a central limit theorem for convexity: It shows that Minkowski sums of arbitrary bounded sets are increasingly close to their convex hull as the number of terms in the sum increases. This produces a priori bounds on the duality gap of separable optimization problems. We use these results to show that several classical sparsity constrained optimization problems have low duality gaps in meaningful data settings.

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MS26

Invexification of Non-Linear Least-Squares Problems

We consider non-convex optimization problems involving a non-linear least-squares objective. We introduce a novel regularization framework whose corresponding objective function is not only provably invex, but it also satisfies the highly desirable Polyak-Lojasiewicz inequality for any choice of the regularization parameter. We then show that, under reasonable assumptions, gradient descent applied to the regularized problem converges exponentially fast to a solution for which the original unregularized objective value has a small sub-optimality. We give explicit bounds to show that such sub-optimality can be made arbitrarily small by directly controlling the regularization parameter. Although our novel framework is entirely different from the classical Tikhonov-type regularizations, an interesting connection is established for the special case of under-determined linear least-squares. In particular, we show that gradient descent applied to our regularized problem converges to the same solution as the ridge regression problem. Numerical experiments corroborate our theoretical results and demonstrate the method's performance in practical situations.

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MS26

AI-SARAH: Adaptive and Implicit Stochastic Recursive Gradient Methods

We present an adaptive stochastic variance reduced method with an implicit approach for adaptivity. As a variant of SARAH, our method employs the stochastic recursive gradient yet adjusts step-size based on local geometry. We provide convergence guarantees for finite-sum minimization problems and show a faster convergence than SARAH can be achieved if local geometry permits. Furthermore, we propose a practical, fully adaptive variant, which does not require any knowledge of local geometry and any effort of tuning the hyper-parameters. This algorithm implicitly computes step-size and efficiently estimates local Lipschitz smoothness of stochastic functions. The numerical experiments demonstrate the algorithm's strong performance compared to its classical counterparts and other state-of-the-art first-order methods.

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MS27

Criteria for Multi-Marginal Maximal Monotonicity

Motivated by multi-marginal optimal transport, we discuss aspects of its underlying monotone and convex analytic structure. We review recent extensions of classical maximal monotonicity and convex analysis into multi-marginal settings. We point out several open questions as well as partial resolutions and examples. In particular, we focus on an extension of Mintys characterization of maximal monotonicity and a generalization of the maximal monotonicity of the convex subdifferential.

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MS27

The Difference Vectors for Convex Sets and a Resolution of the Geometry Conjecture

Projection operators and associated projection algorithms are fundamental building blocks in fixed point theory and optimization. In this talk, I will survey recent results on the displacement mapping of the right-shift operator and sketch a new application deepening our understanding of the geometry of the fixed point set of the composition of projection operators in Hilbert space. Based on joint works with Salha Alwadani, Julian Revalski, and Shawn Wang.

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MS27

Convex Optimization with Sparse, Positive Semidefinite Matrices for Big Data

A traditionally successful approach to those problems described in the title is an application of clique decompositions from sparse matrix theory. Here, we take an alternative approach by viewing sparse semidefinite programming problems (and more generally nonlinear optimization problems) as problems over sparse matrix cones. Unlike the cones of symmetric positive semidefinite matrices, such cones are very rarely self-dual. We identify a class of conic optimization problems called *homogeneous chordal cones*. These are regular convex cones whose automorphism groups act transitively in the interior of the cone and at the same time the members of the cone can be expressed as the nonzero elements of a cone of symmetric positive semidefinite matrices with chordal sparsity pattern. This class of convex cones lie strictly between SDPs and Homogeneous Cone Programming problems. We illustrate how convex optimization problems based on homogeneous chordal cones provide a better generalization of Second Order Cone Programming problems compared with SDPs and better ways of exploiting the related special structures in many special cases as well as in some more general settings of nonlinear optimization problems.

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MS28

A Convex Form that is Not a Sum of Squares

Every convex homogeneous polynomial (or form) is nonnegative. A natural question, raised by Parrilo, is whether every convex form has the stronger property of being a sum of squares. Blekherman subsequently showed that convex forms that are not sums of squares exist via a nonconstructive argument, but until now no explicit examples seem to be known. In this talk I will discuss an explicit example of a convex form of degree four in 272 variables that is not a sum of squares. The form is related to the Cauchy-Schwarz inequality over the octonions. I will also discuss connections between this question and the quality of sum-of-squares-based relaxations of polynomial optimization problems over the sphere.

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MS29

Analysis of Adaptive Stochastic Optimization Methods via Submartingales

We will review recent advances in the analysis of complexity bounds of stochastic line search, trust region and regularized Newton methods for nonconvex optimization. Expected complexity bounds and high probability results will be discussed.

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MS29

SGD for Structured Nonconvex Functions: Learning Rates, Minibatching and Interpolation

We provide several convergence theorems for SGD for two large classes of structured non-convex functions: (i) the Quasar (Strongly) Convex functions and (ii) the functions satisfying the Polyak-Lojasiewicz condition. Our analysis relies on the Expected Residual condition which we show is a strictly weaker assumption as compared to previously used growth conditions, expected smoothness or bounded variance assumptions. We provide theoretical guarantees for the convergence of SGD for different step size selections including constant, decreasing and the recently proposed stochastic Polyak step size. In addition, all of our analysis holds for the arbitrary sampling paradigm, and as such, we are able to give insights into the complexity of minibatching and determine an optimal minibatch size. In particular we recover the best known convergence rates of full gradient descent and single element sampling SGD as a special case. Finally, we show that for models that interpolate the training data, we can dispense of our Expected Residual condition and give state-of-the-art results in this setting.

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MS30

An Interior-Point Method for Low-Rank Semidefinite Programming with Application to Truss Topology Optimization

General purpose algorithms and software for semidefinite optimization are unsuitable to solve problems of very large dimension, often appearing in applications. In order to be able to solve such problems, one has to use their data structure, if available. In this talk, we focus on SDP problems with low-rank solutions. Within a standard framework of an interior-point algorithm, we propose to solve the (Schur complement) linear systems by a preconditioned conjugate gradient method. We present a new preconditioner, tailored to the low-rank structure of the solution. To demonstrate the efficiency of the new method, we solve large to very large scale SDP problems from structural optimization with either a rank-one solution or with an "approximate low-rank solution. In both cases, our Matlab software clearly outperforms available general purpose SDP software.

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MS30

Stability Verification of Dynamical Systems Controlled by Neural Networks using Semidefinite Programming

This presentation makes two observations on stability and performance verification of nonlinear dynamical systems controlled by neural networks. First, we show that the stability and performance of a polynomial dynamical system controlled by a neural network with semialgebraically representable activation functions (e.g., ReLU) can be certified by convex semidefinite programming. The result is based on the fact that the semialgebraic representation of the activation functions and polynomial dynamics allows one to search for a Lyapunov function using polynomial sum-of-squares methods. Second, we remark that even in the case of a linear system controlled by a neural network with ReLU activation functions, the problem of verifying asymptotic stability is undecidable.

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MS30

A Relaxed Interior Point Method for Low-Rank Semidefinite Programming Problems with Applications to Matrix Completion

A new relaxed variant of interior point method for low-rank semidefinite programming problems is proposed in this paper. The method is a step outside of the usual interior point framework. In anticipation to converging to a low-rank primal solution, a special nearly low-rank form of all primal iterates is imposed. To accommodate such a (restrictive) structure, the first order optimality conditions have to be relaxed and are therefore approximated by solving an auxiliary least-squares problem. The relaxed interior point framework opens numerous possibilities how primal and dual approximated Newton directions can be computed. In particular, it admits the application of both the first- and the second-order methods in this context. The convergence of the method is established. A prototype implementation is discussed and encouraging preliminary computational results are reported for solving the SDP-reformulation of matrix-completion problems.

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MS30

Primal-Dual Augmented Lagrangian Method for the Solution of Convex Semidefinite Programming Problems with Applications in Structural Optimization

A primal-dual Augmented Lagrangian (PDAL) method for the solution of convex semidefinite programs is presented. The method is based on the Penalty-Barrier-Multiplier (PBM) idea introduced for semidefinite programming by M. Zibulevsky in 2000. The PDAL method extends the original concept in several ways. When applying penalty-barrier-functions in the context of semidefinite programming the computational complexity for assembling the Hessian of the Augmented Lagrangian is one order of magnitude higher than in comparable approaches using modified barrier functions or the logdet-function. We show that this disadvantage can be fully eliminated, when combining the PBM concept with iterative solvers for the solution of the arising Newton systems. The second point is that instead of a purely primal iteration, a primal dual-update is added. It is shown that the primal dual updates do not only decrease the number of Newton systems to be solved, but also add to the stability of the method. Third, is is shown that the structure of the primal-dual system to be solved in each iteration is very similar to systems which appear in the context of interior point methods. This is why it is possible to employ preconditioners from this context. It will be shown that this is in particularly attractive when SDPs are solved for which the rank of the primal matrix variable is known to be of low-rank. Numerical examples include linear and nonlinear problems from the area of structural optimization.

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MS31

Constrained and Composite Optimization via Adaptive Sampling

Variance reduction via adaptive sampling strategies has recently received much attention for solving unconstrained stochastic optimization problems. In this talk, we extend these schemes for solving constrained and composite optimization problems via the proximal gradient method. We establish global theoretical convergence results for an optimization method based on these schemes and present numerical experiments on logistic regression problems.

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MS31

Gradient Sampling Methods with Inexact Subproblem Solutions and Gradient Aggregation

Gradient sampling methods have proved to be effective for solving nonconvex, nonsmooth optimization problems. In this talk, we present two improvements that offer practical benefits while maintaining convergence guarantees, thus allowing for the more efficient solution of large-scale problems. The first is a strategy for allowing the arising quadratic optimization (QP) subproblems to be solved inexactly. The second is a scheme for employing gradient aggregation in order to limit the size of the subproblems that need to be solved in the first place. We demonstrate using the NonOpt software that these algorithmic modifications lead to computational savings.

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MS31

Random Embeddings and their Application to Optimization Algorithms

We first show that sparse random matrices (hashing ensembles with one or more non-zeros per column) have subspace embedding properties that are optimal in the sketching dimension. We then show the implications of this result for the efficient solution of least squares problems, in reducing the dimension of the observational or parameter spaces; and more generally, for random subspace variants of well known nonconvex optimization algorithms. Global rates of convergence as well as some numerical experiments are presented.

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MS32

Recent Trends in Adaptive Regularisation under Inexact Evaluations for Nonconvex Optimisation

Within the context of nonconvex unconstrained and inexpensively-constrained optimisation, a class of adaptive regularisation methods under inexact function and derivatives evaluations is presented. At variance with the ARC framework, the underlying algorithm is not limited to refer to the cubic model, allowing for the use of potentially higher degrees to search for arbitrary order optimality points. At each iteration, it features an adaptive mechanism for determining the inexactness which is needed to compute objective function values and derivatives, in order to preserve the complexity results of its counterpart with exact evaluations. Sharp global evaluation complexity bounds, assuming that the right accuracy level in function and derivatives estimates is deterministically achievable, are derived and hold for any model degree and any order of optimality, thereby generalising known results for first and second-order versions of the method. High probability and stochastic complexity bounds are also shown. For lower orders, preliminary numerical tests are finally reported.

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MS32

Detection of Iterative Adversarial Attacks via Counter Attack

Deep neural networks (DNNs) have proven to be powerful tools for processing unstructured data. However for high-dimensional data, like images, they are inherently vulnerable to adversarial attacks. Small, almost invisible perturbations added to the input can be used to fool DNNs. Various attacks, hardening methods and detection methods have been introduced in recent years. Notoriously, Carlini-Wagner (CW) type attacks computed by iterative minimization belong to those that are most difficult to detect. In this work, we demonstrate that the same minimization problems solvable by the projected subgradient method can by used as detectors themselves. Thus, in some sense we show that one can fight fire with fire. This work also outlines a mathematical proof that under certain assumptions this detector provides asymptotically optimal separation of original and attacked images. In numerical experiments, we obtain AUROC values up to 99.73% for our detection method. This distinctly surpasses state of the art detection rates for CW attacks from the literature. We also give numerical evidence that our method is robust against the attackers choice of the method of attack.

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MS32

A Newton-Mr Algorithm with Complexity Guarantee for Non-Convex Problems

Classically, the conjugate gradient (CG) method has been the dominant solver in most inexact Newton-type methods for unconstrained optimization. In this talk, we consider replacing CG with the minimum residual method (MINRES), which is often used for symmetric but possibly indefinite linear systems. We show that MINRES has an inherent ability to detect negative-curvature directions. Equipped with this advantage, we discuss algorithms, under the general name of Newton-MR, which can be used for optimization of general non-convex objectives, and that come with favourable complexity guarantees. We also give numerical examples demonstrating the performance of these methods for large-scale non-convex machine learning problems.

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MS32

A Novel Class of Second-Order Stochastic Optimization Methods

We propose a class of stochastic optimization methods, named LSOS, where Newton, inexact Newton and limited-memory quasi-Newton directions are used together with line-search techniques. Almost sure convergence of the sequence of iterates holds for all the LSOS variants; furthermore, for finite-sum problems, linear convergence of the expected objective function error is obtained when stochastic L-BFGS Hessian approximations and Lipschitz-continuous unbiased gradient estimates are used. Numerical experiments show that our methods are highly competitive with state-of-the art stochastic optimization methods.

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MS33

Compact Mixed-Integer Programming Relaxations in Quadratic Optimization

We present a technique for producing valid dual bounds for nonconvex quadratic optimization problems. The approach leverages an elegant piecewise linear approximation for univariate quadratic functions due to Yarotsky, formulating this (simple) approximation using mixed-integer programming. Notably, the number of constraints, binary variables, and auxiliary continuous variables used in this formulation grows logarithmically in the approximation error. Combining this with a diagonal perturbation technique to convert a nonseparable quadratic function into a separable one, we present a mixed-integer convex quadratic relaxation for nonconvex quadratic optimization problems. We study the strength of our formulation in terms of sharpness and the tightness of our approximation. Further, we show that our formulation represents feasible points via a Gray code. We close with computational results on box-constrained quadratic optimization problems, showing that our technique can outperform existing approaches in terms of solve time and dual bounds.

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MS33

Lifting Convex Inequalities for Bipartite Bilinear Programming

We design new valid convex inequalities for QCQPs via the technique of lifting. Our first main result is to show that for sets described using one bipartite bilinear quadratic constraint together with bounds, it is always possible to lift a seed inequality that is valid for a restriction obtained by fixing variables to their bounds, and the lifting is accomplished using affine functions of the fixed variables. Sequential lifting involves solving a non-convex nonlinear problem to lift one variable at a time. This can be computationally very prohibitive. Therefore, we develop a framework for approximate sequence independent lifting of seed inequalities for separable bipartite bilinear quadratic constraint. We study a simple case where the coefficients form a minimal cover with respect to right-hand-side (minimal cover defined in an analogous fashion as in integer programming). For this set, we describe a bilinear cover inequality, which is second order cone representable. We prove various results about it, such as showing a constant-factor approximation of the convex hull of the original set. We are able to construct a two-slope subadditive function that upper bounds the lifting function. Using this subadditive function we are able to lift fixed variable pairs in a closed form, thus deriving a lifted bilinear covering inequality that are valid inequalities for general separable bipartite bilinear quadratic constraints together with box constraints.

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MS33

Convexification for MIQPs and other Recent Advances in the BARON Project

We report recent developments in the BARON project, including work with Carlos Nohra and Arvind Raghunathan on the global optimization of mixed-integer quadratic programs for which we present and theoretically analyze quadratic relaxations in the original variable space. We report extensive computational results with BARON on a variety of problems, including general mixed-integer nonlinear programs, portfolio optimization problems, and quadratic assignment problems.

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MS34

Structures of Local Minima in K-Means and Mixture Models

Maximum likelihood estimation of mixture models poses non-convex problems. Standard algorithms such as EM generally converge to a spurious local minimizer, both in theory and practice. In this talk, we present two results on the structures of these local minima. For a mixture of two symmetric components, we show that all local minima are globally optimal, and EM converges to a global optimum from random initialization. This result applies to a broad class of log-concave mixture problems including mixtures of Gaussians and linear regressions. Our analysis highlights the non-convergence of EM in Euclidean distance, necessitating the consideration of other metrics. For a mixture of more than two components, spurious local minima provably exist. One such local minimizer puts multiple centers at one true component, and another center in the middle of multiple true components. We prove that this is essentially the only type of spurious local minima under a separation condition. Consequently, EM is guaranteed to converge to a solution that at least partially identify the true mixture model. We will discuss further algorithmic implications of these results for over-parameterization.

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MS34

An Inertial Block Majorization Minimization Framework for Nonsmooth Nonconvex Optimization

This talk is based on the joint works with D.N Phan, N. Gillis, M. S. Ang, and O. Vu thanh. In this talk, we introduce TITAN, a novel inertial block majorization minimization framework for nonsmooth nonconvex optimization problems. TITAN is a block coordinate method (BCM) that embeds inertial force to each majorization-minimization step of the block updates. The inertial force is obtained via an extrapolation operator that subsumes heavy-ball and Nesterov-type accelerations for block proximal gradient methods as special cases. By choosing various surrogate functions, such as proximal, Lipschitz gradient, Bregman, quadratic, and composite surrogate functions, and by varying the extrapolation operator, TITAN produces a rich set of inertial BCMs. We study sub-sequential convergence as well as global convergence for the generated sequence of TITAN. We illustrate the effectiveness of TITAN on two important machine learning problems, namely matrix completion problem and min-vol nonnegative matrix factorization problem.

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MS34

Convex Clustering

Recently, convex clustering models based on sum-of-norms have been proposed. The perfect recovery properties of the convex clustering model with uniformly weighted all pairwise-differences regularization have been proved by Panahi et al. in 2017. In this talk, we present sufficient conditions for the perfect recovery of the general weighted convex clustering model, which include and improve existing theoretical results as special cases. We also develop a semismooth Newton based augmented Lagrangian method for solving large-scale convex clustering problems. Extensive numerical experiments on both simulated and real data demonstrate that our algorithm is highly efficient and robust for solving large-scale problems. Moreover, the experiments also show the superior performance and scalability of our algorithm comparing to the existing first-order methods. In particular, our algorithm is able to solve a convex clustering problem with 200,000 points in 3-dimension in about 6 minutes.

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MS34

Convex Relaxation for Overlapping Community Detection

Community detection (aka graph clustering) is a common unsupervised learning problem which finds applications in diverse domains such as computational biology, social network analysis, and document classification. Stochastic Blockmodel (SBM) is a popular generative model for random graphs used to perform theoretical analyses of community detection algorithms. However, SBM assumes that the communities do not overlap. Therefore, we consider a generalization of SBM, called Mixed Membership Stochastic Blockmodel (MMSB), which allows overlapping communities. In this work, we provide a simple, efficient, convex-optimization based, provable community detection algorithm which takes as input a weighted graph, and provide recovery guarantees if the graph is generated according to MMSB. Our algorithm involves only one tuning parameter (which is fairly standard, in that it also appears in most other competing algorithms), and our theoretical analysis dispenses the requirement of so-called pure nodes.

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MS35

SPRING: A Stochastic Algorithm for Non-smooth Non-convex Optimization

Many problems in image processing can be formulated as large-scale, complex optimization problems. Often non-convex, non-smooth, and involving multiple regularizers, few optimization algorithms can tackle these problems. In this talk, we introduce SPRING, a stochastic extension of the celebrated PALM algorithm that can efficiently solve a broad class of non-smooth non-convex problems. We show that SPRING achieves state-of-the-art convergence rates on non-convex problems, even achieving oracle complexity lower-bounds in certain settings, and SPRING achieves state-of-the-art performance on several large-scale imaging problems.

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MS35

Convex-Concave Backtracking for Inertial Bregman Proximal Gradient Algorithms in Non-Convex Optimization

Backtracking line-search is an old yet powerful strategy for finding better step size to be used in proximal gradient algorithms. The main principle is to locally find a simple convex upper bound of the objective function, which in turn controls the step size that is used. In case of inertial proximal gradient algorithms, the situation becomes much more difficult and usually leads to very restrictive rules on the extrapolation parameter. In this talk, we show that the extrapolation parameter can be controlled by locally finding also a simple concave lower bound of the objective function. This gives rise to a double convex-concave backtracking procedure which allows for an adaptive and optimal choice of both the step size and extrapolation parameters. We apply this procedure to the class of inertial Bregman proximal gradient methods, and prove that any sequence generated converges globally to critical points of the function at hand. Numerical experiments on a number of challenging non-convex problems in image processing and machine learning were conducted and show the power of combining inertial step and double backtracking strategy in achieving improved performances.

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MS35

Expanding Boundaries of Gap Safe Screening

A powerful strategy to boost the performance of sparse optimization algorithms is known as safe screening: it allows the early identification of zero coordinates in the solution, which can then be eliminated to reduce the problem's size and accelerate convergence. In this work, we extend the existing Gap Safe screening framework by relaxing the global strong-concavity assumption on the dual cost function. Instead, we exploit local regularity properties, that is, strong concavity on well-chosen subsets of the domain. The non-negativity constraint is also integrated to the existing framework. Besides making safe screening possible to a broader class of functions that includes beta-divergences (e.g., the Kullback-Leibler divergence), the proposed approach also improves upon the existing Gap Safe screening rules on previously applicable cases (e.g., logistic regression).

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MS35

Stochastic Finite Difference Methods for Smooth Convex Optimization

In this talk I will discuss a class of methods for which the direction of descent is an approximation of the gradient in a low-dimensional random subspace. The approximation is two-fold, one coming from the projection onto a random subspace and the other from the use of finite-differences to calculate the directional derivatives. Commonly used methods that fall under this framework include spherical smoothing, coordinate descent, and even discretized gradient descent. I will provide convergence analysis and rates under varying assumptions on the objective function, the step-size, and the discretization mesh. This is a joint work with D. Kozak, C. Molinari and L. Rosasco.

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MS36

Plug-and-Play Superiorization for CT Image Reconstruction

Superiorization is an optimization heuristic in which the iterates of a feasibility-seeking (”basic”) algorithm are perturbed in every iteration, according to some secondary criterion. If the basic algorithm satisfies certain properties (”perturbation resilience”) and the size of the perturbations are controlled, it can be shown that the superiorized version of the algorithm converges to solutions that are equally constraints-compatible to those produced by the basic algorithm. These solutions can also expected to be superior (but not necessarily optimal) with respect to the secondary criterion. Traditionally the perturbations are chosen to be non-ascending directions of some target function, such as total variation. There may be instances, however, where it is beneficial to introduce perturbations that are not of this form; for example, based on the output of an image denoiser or a neural network. We therefore propose a “plug-and-play’ framework for superiorization which allows for perturbations of this type. We demonstrate the efficacy of the approach on the problem of low-dose and sparse-view CT imaging, using perturbations generated by both a popular denoising algorithm and a pretrained convolutional neural network.

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MS36

A Feasibility Study of a Hyperparameter Tuning Approach to Automated Inverse Planning in Radiotherapy

In current practice, radiotherapy inverse planning requires treatment planners to modify multiple parameters in the objective function to produce clinically acceptable plans. Due to the manual steps in this process, plan quality can vary widely depending on the planning time available and the planners skills. The purpose of this study is to automate the inverse planning process to reduce the planner’s active planning time while maintaining plan quality. We propose a hyperparameter tuning approach for automated inverse planning, where a treatment plan utility is maximized with respect to the limit dose parameters and weights of each organ-at-risk (OAR) objective. Using five patient cases, we investigated the impact of the choice of dose parameters, random and Bayesian search methods, and utility function form on planning time and plan quality. For given parameters, the plan was optimized in RayStation, using the scripting interface to obtain the dose distributions deliverable. The OAR doses in the automatically generated plans were lower than the clinical plans by up to 76.8%. When the OAR doses were larger than the clinical plans, they were still between 0.57% above and 98.9% below the limit doses, indicating they are clinically acceptable. This study demonstrates our hyperparameter tuning framework for automated inverse planning can significantly reduce the treatment planner’s planning time with plan quality that is similar to or better than manually generated plans.

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MS37

Asymptotic Network Independence in Distributed Stochastic Gradient Methods

We provide a discussion of several recent results which, in certain scenarios, are able to overcome a barrier in distributed stochastic optimization for machine learning (ML). Our focus is the so-called asymptotic network independence property, which is achieved whenever a distributed method executed over a network of n nodes asymptotically converges to the optimal solution at a comparable rate to a centralized method with the same computational power as the entire network. We explain this property through an example involving the training of ML models and sketch a short mathematical analysis for comparing the performance of distributed stochastic gradient descent (DSGD) with centralized SGD.

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MS37

Distributed Approximate Methods of Multipliers for Convex Composite Optimization

In many engineering scenarios, a network of agents needs to cooperatively find a common decision that minimizes the sum of local objective functions. A large body of distributed optimization algorithms has been proposed to solve this problem. However, relatively few of them are able to address general convex and nonsmooth local objective functions. This talk considers such a problem on an arbitrarily connected network, where each local objective function is composite, i.e., the sum of a smooth component function and a nonsmooth one. To address the problem, a general Approximate Method of Multipliers (AMM) is developed, which attempts to approximate the Method of Multipliers by virtue of a surrogate function with numerous options. We then design the surrogate function in various ways, leading to different realizations of AMM that enable distributed implementations over the network. We demonstrate that AMM generalizes over ten state-of-the-art distributed optimization algorithms, and certain specific designs of its surrogate function introduce a variety of brand-new algorithms to the literature. Furthermore, we show that AMM is able to achieve an O(1/k) rate of convergence to optimality, and the convergence rate becomes linear when the problem is locally restricted strongly convex and smooth. Such convergence rates provide stronger convergence results to many prior methods that can be viewed as specializations of AMM.

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MS37

Distributed Optimization and Its Application in Smart Grid

Distributed optimization algorithms solve large-scale optimization problems through collaboration among multiple agents. Compared with classical centralized optimization algorithms, distributed optimization algorithms are more flexible, convenient and efficient. Distributed optimization algorithms are widely used in power systems, transportation systems, cyber-physical systems and other fields. This talk first reviews and summarizes the existing distributed optimization algorithms; next, for the optimal collaborative control of distributed energy in smart grids, two distributed collaborative optimization algorithms are proposed, and the convergence of the algorithms is rigorously proved theoretically. At the same time, it was verified in IEEE-39 bus system.

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MS37

Decentralized Stochastic Quasi-Newton Methods

We study decentralized stochastic quasi-Newton methods for minimizing a finite sum of objectives over a network. First, we establish a general framework that incorporates quasi-Newton approximations with variance reduction so as to achieve fast convergence. With a fixed step size, we show the condition under which the general framework linearly converges to the exact solution. Second, we propose two fully decentralized quasi-Newton approximations, limited-memory DFP and limited memory BFGS, to locally construct the estimators of Hessian inverse. Both quasi-Newton approximations are proven to satisfy the condition of exact linear convergence. Numerical experiments demonstrate that the proposed quasi-Newton methods are faster than the existing decentralized stochastic first-order algorithms.

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MS38

Efficient Optimization of Black Box Problems with Computationally Expensive Constraints

We develop several approaches for the optimization of black-box problems whose objective and constraint function evaluations are obtained by running time-consuming independent simulations, i.e., we can first evaluate the constraint to assess the feasibility of a proposed solution before committing to spending more time on evaluating the objective function. Gaussian process models are employed to approximate the objective and the constraints. We consider several adaptive sampling strategies for iteratively selecting new evaluation points. These strategies exploit uncertainty estimates of the constraint and objective function value predictions that are provided by the Gaussian process models. We analyze the advantages as well as potential pitfalls of our constraints first approach on illustrative test problems.

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MS38

PDFO: a Cross-Platform MATLAB/Python Interface for Powell's Derivative-Free Optimization Solvers

Late Professor M. J. D. Powell designed five derivative-free optimization algorithms, namely COBYLA, UOBYQA, NEWUOA, BOBYQA, and LINCOA. The algorithms were implemented in FORTRAN 77 and therefore may not be easily accessible to some users. This talk aims to introduce the PDFO (Powells Derivative-Free Optimization) package, which is developed to provide both Python and MATLAB interfaces to Powell's code. With PDFO, users can call each of Powell's algorithm directly based on their own choice. Alternatively, if the user does not specify any algorithm, the package can also select one automatically based on the problem characteristics. When a problem can be solved by multiple algorithms (for example, an unconstrained problem can be solved by all the five algorithms), the selection is made based on experimental results on the CUTEst problems. We will also share some observations about the behavior of Powell's algorithms on these problems. This talk is based on a part of a Ph.D. research funded by the RGC of Hong Kong under the Hong Kong Ph.D. Fellowship Scheme (ref. PF18-24698).

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MS38

A Derivative-Free Approach for Structured Optimization Problems

Structured optimization problems are ubiquitous in fields like data science and engineering. The goal in structured optimization is using a prescribed set of points, called atoms, to build up a solution that minimizes or maximizes a given function. In the present talk, we want to minimize a black-box function over the convex hull of a given set of atoms, a problem that can be used to model a number of real-world applications. We focus on problems whose solutions are sparse, i.e., solutions that can be obtained as a proper convex combination of just a few atoms in the set, and propose a suitable derivative-free inner approximation approach that nicely exploits the structure of the given problem. This enables us to properly handle the dimensionality issues usually connected with derivative-free algorithms, thus getting a method that scales well in terms of both the dimension of the problem and the number of atoms. We analyze global convergence to stationary points. Finally, we report numerical results showing the effectiveness of the proposed method.

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MS38

Optimization by Space Transformation and Decomposition

We introduce a space transformation framework for unconstrained optimization of an objective function that is smooth but not necessarily convex. At each iteration of the framework, the gradient of f is mapped by a forward transformation to an auxiliary (possibly lifted) space, in which a model is established based on the transformed gradient and a step is obtained by minimizing this model. A backward transformation then maps the step back to the original space, where the iterate is updated accordingly. Using a trust-region globalization scheme, and by inspection of the consistency between the forward and backward transformations, the framework is guaranteed to converge globally to first-order criticality with a $O(\epsilon^{-2})$ worst-case iteration complexity to reach a gradient with norm smaller than ϵ. The complexity is improved to $O(\epsilon^{-1})$ and $O(\log(\epsilon^{-1}))$ when the objective function is convex and strongly convex respectively. The space transformation framework can be directly specialized to a parallel space decomposition framework for nonlinear optimization, which can be regarded as an extension of the parallel Schwarz domain decomposition method for PDEs and linear systems. Meanwhile, it can be specialized to analyze trust-region methods when the gradient of the objective function is evaluated inaccurately. Our work provides a unified view on these two seemingly unrelated topics.

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MS39

Robust Optimization with Side Data

We introduce and solve the problem of minimizing a cost function subject to constraints that depend on an uncertain parameter, given historical data on the parameter, including side data. We develop two approaches to solving this problem, both involving replacing the uncertain constraints by constraints evaluated at data points. Both approaches are at least as tractable as the original problem. We show that the degree of suboptimality and degree of constraint violation of the decision produced by both approaches converges almost surely to zero. We show that for both approaches, varying a single parameter controls the tradeoff between suboptimality and constraint violation, and we propose a cross-validation scheme for choosing the parameter to enforce the desired tradeoff. We implement both approaches and the cross-validation scheme on a wide range of computational examples and observe that both approaches produce a satisfactory decision and that the cross-validation scheme is effective in choosing the tradeoff between suboptimality and constraint violation. We also combine both approaches with prior work to extend them to the setting in which both the objective and constraints are uncertain, forming two tractable theories of optimization under uncertainty with side data (joint work with Nihal Konduri) .

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MS39

Correlation Robust Influence Maximization

We propose a distributionally robust model for the influence maximization problem. Unlike the classic independent cascade model this model's diffusion process is adversarially adapted to the choice of seed set. We show that the worst-case influence function can be efficiently computed, and though the optimization problem is NP-hard, a 1-1/e approximation guarantee holds. Beyond the key computational advantages, we also highlight the extent to which the independence assumption may cost optimality, and provide insights from numerical experiments comparing the adversarial and independent cascade model.

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MS39

An Adaptive Robust Optimization Model for Parallel Machine Scheduling

Real-life parallel machine scheduling problems can be characterized by: (i) limited information about the exact task durations at the time of their scheduling, and (ii) an opportunity to reschedule the remaining tasks each time a task completed its processing and a machine becomes idle. Robust optimization is the natural methodology to cope with the fisrt characteristic of duration uncertainty, yet the existing literature on robust scheduling does not explicitly consider the second characteristic which is the possibility to adjust decisions as more information about the tasks' durations is revealed. This is despite the fact that re-optimizing the schedule every time new information becomes available is a standard practice. In this paper, we develop a scheduling approach that takes into account, at the beginning of the planning horizon, the possibility that scheduling decisions can be adjusted. We demonstrate that the suggested approach can lead to better here-and-now decisions. To that end, we develop the first mixed integer linear programming model for adjustable robust scheduling, where we minimize the worst-case makespan. Using this model, we show via a numerical study, that adjustable scheduling leads to solutions with better and more stable makespan realizations compared to static approaches.

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MS39

Optimal Elective Care Scheduling during the Sars-CoV-2 Pandemic

The COVID-19 pandemic has seen dramatic demand surges for inpatient care that have placed a severe strain on health systems worldwide. As a result, policy makers are faced with the challenge of managing scarce hospital capacity so as to reduce the backlog of non-COVID-19 patients whilst maintaining the ability to respond to any potential future increases in demand for COVID-19 care. In this paper, we propose an optimization-based prioritization scheme that models individual patients as Markov decision processes (MDPs) whose states encode the patient's health (emergency/non-emergency, recovered or deceased) and treatment state (waiting for treatment, in general & acute or in critical care), whose actions describe the treatment options (move to general & acute or to critical care, discharge from hospital) and whose transition probabilities characterize the stochastic evolution of the patient's health. The individual patients' MDPs are coupled through constraints on the available resources, such as hospital beds, doctors and nurses. We show that near-optimal solutions to the emerging weakly coupled MDP problem can be found through a fluid relaxation that gives rise to a linear program whose size grows gracefully in the problem dimensions.

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MS40

More Efficient and Flexible Flag-SOS Hierarchies coming from Polynomial Optimization

Flag Algebras, i.e. gluing-algebras of limit operators describing the densities of partially labelled sub-graphs, were first introduced by Razborov in 2007 as a powerful tool for problems in extremal combinatorics. Recently Raymond et al. investigated the connections between Flag-SOS and limits of symmetric problems in polynomial optimization, describing an alternative way to derive these algebras. We take a closer look at the symmetry of this problem, deriving a more efficient equivalent hierarchy. We then describe a natural way to extend Flag-Algebras to model limits of graphs that are not dense. This results in new hierarchies solving problems such as the problem of maximizing the edge density of a graph while avoiding C4.

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MS40

On the Finite Convergence of Sum-of-Squares Hierarchies for the Maximum Stable Set Problem

Given a graph G, its stability number is the cardinality of the largest subset of vertices without edges between them. Computing the stability number is an NP-hard problem and some approximations via semidefinite optimization have been developed. One of them is a hierarchy proposed by de Klerk and Pasechnik by following an idea given by Parrilo for approximating problems over the copositive cone. One open question asks for the finite convergence of this hierarchy. We prove finite convergence for the class of graphs without critical edges. Our analysis relies on exploiting a link to the Lasserre hierarchy for the Motzkin-Straus formulation and using a known sufficient condition for its finite convergence. As an application we can show that deciding whether a standard quadratic problem has finitely many global minimizers is hard. This is joint work with Monique Laurent

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MS40

Hard Combinatorial Problems, Doubly Nonnegative Relaxations, Facial Reduction, and Alternating Direction Method of Multipliers

We look at doubly nonnegative relaxations for several classes of hard problems. We present a successful approach based on using facial reduction and a splitting of variables. We look at: second lifting for max-cut, as well as the quadratic assignment and graph partitioning problems. We show that the Slater constraint qualification, strict feasibility, fails for all these problems. Rather than resulting in theoretical and numerical difficulties, we show how to use facial reduction, FR, to regularize, reduce the dimension of the problem, and provide a natural splitting of the variables. Our numerical results illustrate that our approach provably solves the max-cut problem to optimality, generically (on random problems).

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MS40

Discrete Semidefinite Programming Techniques for the Quadratic Traveling Salesman Problem

The Quadratic Traveling Salesman Problem (QTSP) is the problem of finding a Hamiltonian cycle in a graph that minimizes the quadratic cost among pairs of arcs that are traversed in succession. We present two discrete semidefinite programming (SDP) formulations of the QTSP that both enjoy an algebraic origin. To solve the QTSP as a discrete SDP, we extend the well-known Chvtal-Gomory procedure for integer linear programming to the class of integer SDP problems. We show that the Chvtal-Gomory cuts for the QTSP have a familiar combinatorial structure that can be exploited in a branch-and-cut algorithm. Our algorithm solves medium-size QTSP instances to optimality using a limited number of these cuts. Our work is in line with the recent interest in discrete semidefinite programming and contributes to this promising field in both theory and applications.

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MS41

Sum-of-Squares Proofs of Logarithmic Sobolev Inequalities on Finite Markov Chains

Logarithmic Sobolev inequalities play an important role in understanding the mixing times of Markov chains on finite state spaces. It is typically not easy to determine, or indeed approximate, the optimal constant for which such inequalities hold. In this paper, we describe a semidefinite programming relaxation for the logarithmic Sobolev constant of a finite Markov chain. This relaxation gives certified lower bounds on the logarithmic Sobolev constant. Numerical experiments show that the solution to this relaxation is often very close to the true constant. Finally, we use this relaxation to obtain a sum-of-squares proof that the logarithmic Sobolev constant is equal to half the Poincar constant for the specific case of a simple random walk on the odd n-cycle, with n in 5,7,...,21. Previously this was known only for n=5 and even n.

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MS41

A Common Framework for SOS Hierarchies of Upper and Lower Bounds

We provide a common framework to interpret the two SOS-based hierarchies of upper and lower bounds for the polynomial optimization problem $\min\{f(x) : x \in K\}$. Namely, fix an arbitrary Borel measure μ whose support is the set of feasible solutions. Then step-d of the SOS-hierarchy of upper bounds is searching for a (positive) density w.r.t. μ which is an SOS polynomial p of degree $2d$, and which minimizes $\int f\, p\, d\mu$. On the other hand, step-d of the SOS-based hierarchy of lower bounds is searching for a *signed* density q (w.r.t. μ) which is a degree-$2d$ polynomial whose coefficients have a certain property, and which also minimizes $\int f\, q\, d\mu$.

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MS41

Exact Moment Representation in Polynomial Optimization

We investigate the problem of representation of moment sequences by measures in Polynomial Optimization Problems, consisting in finding the infimum f^* of a real polynomial f on a basic real semialgebraic set. We analyse the exactness of Moment Matrix (MoM) relaxations, dual to the Sum of Squares (SoS) relaxations, which are hierarchies of convex cones introduced by Lasserre to approximate measures and positive polynomials. We show the exactness of MoM relaxation when regularity conditions, known as Boundary Hessian Conditions, hold on the minimizers. When the set of minimizers is finite, we describe a MoM relaxation which involves f^*, and show its MoM exactness. We also show that if the real variety of polar points is finite then the MoM relaxation extended with the polar constraints is exact.

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MS41

Sum-of-Squares Hierarchies for Binary Polynomial Optimization

We consider the hierarchy of sum-of-squares approximations for the problem of computing the minimum value of a polynomial f over the n-dimensional boolean hypercube. This hierarchy provides lower bounds for each order r and is known to be exact at (roughly) order $(n + d)/2$, where d is the degree of f. We provide an asymptotic analysis for the quality of the bound in the regime where the order r is approximately equal to $t * n$ for some scalar t in $[0, 1/2]$, showing that the relative error is in the order $1/2 - \sqrt{t(1-t)}$. Our analysis relies on constructing suitable feasible solutions using polynomial kernels, which we obtain by exploiting symmetry and Fourier analysis on the Boolean cube. A crucial tool is relating the sum-of-squares hierarchy to another hierarchy of measure-based *upper* bounds (also introduced by Lasserre), and to exploit a link to extremal roots of orthogonal polynomials (in this case the Krawtchouk polynomials). Our error analysis in fact also applies to this second hierarchy. This is based on joined work with Monique Laurent.

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MS42

Derivative-Free Trust Region Methods for Unconstrained and Convexly Constrained Multiobjective Optimization

The goal of multiobjective optimization is the identification of one or several acceptable trade-offs between conflicting objective functions. There is a multitude of methods available to treat such problems. However, many real-world multiobjective optimization problems (MOP) require computationally expensive objective evaluations. Consequently, it becomes infeasible to use Genetic Algorithms with large populations. Neither can the gradients or Hessians be approximated efficiently in high dimensional settings for use in traditional derivative-based methods. Instead, we present a flexible trust region framework that is designed to require as few objective function evaluations as possible by using locally accurate, fully linear surrogate models of the true objectives. As in the corresponding scalar framework, convergence to first-order critical points can be proven. In our work, we were heavily inspired by existing trust region methods for MOP. Our main contributions are the integration of convex constraints and the implementation of radial basis function (RBF) surrogate models. The use of RBF models reduces the number of expensive evaluations - from a quadratic to a linear upper bound. We present numerical experiments illustrating their efficacy.

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MS42

Stationarity Conditions and Scalarization in Multiobjective Optimal Control of a Non-Smooth PDE

This talk addresses the multiobjective optimal control of a non-smooth semilinear elliptic PDE with max-type nonlinearity and either $L^2(\Omega)$- or finite dimensional controls. We consider different (Pareto) stationarity systems depending on the control space. The weighted-sum method and the reference point method are compared as two scalarization approaches to calculate Pareto stationary points. In the reference point method, a matrix-free preconditioned L-GMRES approach for a globalized pseudo semismooth Newton method is presented to overcome computational difficulties. Numerical examples are shown to illustrate the capabilities of this approach.

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MS42

Completely Positive Relaxations of Quadratic Problems in a Multiobjective Framework

In a single-objective setting, nonconvex quadratic problems can equivalently be reformulated as convex problems over the cone of completely positive matrices. In small dimensions this cone equals the cone of matrices which are entrywise nonnegative and positive semidefinite, so the convex reformulation can be solved via SDP solvers. Considering multiobjective nonconvex quadratic problems, naturally the question arises, whether the advantage of convex reformulations extends to the multicriteria framework. In this talk, we will see that this approach only finds the supported nondominated points, which can already be found by using the weighted sum scalarization of the multiobjective quadratic problem, i.e. it is not suitable for nonconvex problems.

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MS42

A Bi-Criteria Moving-Target Traveling Salesman Problem under Uncertainty

This study concerns a variant of moving target traveling salesman problem where the number and locations of targets vary with time and realizations of random trajectories. Objectives are to maximize the number of visits to moving targets and to minimize the total travel distance. Employing a linear value function for finding supported Pareto-efficient solutions, we develop a two-stage stochastic programming model. We propose an iterative Randomized Dynamic Programming (RDP) algorithm which converges to a global optimum with probability one. Each iteration in RDP involves a randomized backward and forward recursion stage as well as options for improving any given schedule: swaps of targets and optimization of timing for visits. An integer linear programming (ILP) model is developed to evaluate the performance of RDP against a standard ILP solver on instances of real data for scheduling an environmental surveillance boat to visit ships navigating in the Baltic sea. Due to a huge number of binary variables, the ILP model in practice becomes intractable. For small to medium size data sets, the Pareto-efficiency of solutions found by RDP and ILP solver are equal within a reasonable tolerance; however, RDP is significantly faster and able to deal with large-scale problems in practice.

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MS43

Bilevel Stochastic Programming Problems in a Shape Optimization Context

Stochastic bilevel problems arise from the interplay between two decision makers on different levels of hierarchy where the lower level problem is entered by a random vector. In our context, this models production errors of a shape that has to be optimized due to possible acting forces. We present a deterministic formulation for a bilevel problem under stochastic uncertainty which is based on special risk measures. In particular, structural properties and qualitative stability of the optimal value function of this model under perturbation of the underlying Borel probability measure will be investigated with respect to weak convergence of probability measures. Focusing on a finite number of realizations of an underlying random vector, equivalences to single-level problems are ascertained to conclude with a regularization scheme for bilevel linear problems.

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MS43

Analysis and Numerical Solution of a Bilevel Optimization Problem Arising in Non-Newtonian Fluid Mechanics

This talk is concerned with the optimal control of stationary and instationary, rotationally symmetric, viscoplastic fluid flows in circular pipes. We study the properties of the solution maps of the nonsmooth minimization problems and parabolic variational inequalities that govern the flow of, e.g., Bingham and Casson fluids in circular pipes and use the obtained results to derive stationarity conditions and to design numerical solution algorithms for the optimal control of non-Newtonian flows. The talk concludes with numerical experiments that confirm the theoretical findings.

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MS43

Optimality Conditions in Bilevel Stochastic Linear Optimization

We consider bilevel stochastic linear programs where the leader decides nonanticipatorily, while the follower has complete information. Invoking the underlying geometry, the talk discusses analytical properties of the arising expectation functional and provides sufficient optimality conditions in terms of generalized Hessians.

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MS43

Stability and Sensitivity of Bayesian Optimal Designs

We revisit Bayesian sensor placement problems for PDE models including unknown parameters. More in detail we focus on the A-optimal design problem which corresponds to minimizing the expected mean squared error of the MAP estimator as a function of the measurement setup i.e. the number, position as well as the variance of the measurements. Since the MAP estimator is defined as solution to a (nonlinear) Least squares problem, this naturally leads to a bilevel optimization problem. One popular approach to this problem consists in linearizing the underlying PDE around a reference parameter. This reduces the problem to a convex minimization problem whose solution set depends on the linearization point. In this talk we investigate this dependence proving several stability results and calculate the sensitivity of the measurement setup w.r.t to perturbations.

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MS44

SQP for Equality Constrained Stochastic Optimization

Stochastic gradient and related methods for solving stochastic optimization problems have been studied extensively in recent years. In addition, it has been shown that such algorithms and much of their convergence and complexity guarantees extend in straightforward ways when one considers problems involving simple constraints, such as when one can perform projections onto the feasible region. However, settings with general nonlinear constraints have received less attention, and many of the approaches that have been proposed for solving such problems resort to using penalty or (augmented) Lagrangian methods, which are often not the most effective strategies. In this work, we propose and analyze stochastic optimization methods based on the sequential quadratic optimization (commonly known as SQP) methodology. We discuss advantages and disadvantages of such techniques. This is joint work with Frank E. Curtis, Daniel P. Robinson and Baoyu Zhou.

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MS44

Adaptive Sampling Strategies for Risk-Averse Stochastic Optimization with Constraints

We introduce a solution methodology for risk-neutral and risk-averse stochastic programs with deterministic constraints. Our approach relies on principles from projected gradient descent and sample average approximation algorithms. However, we adaptively control the sample size used in computing the reduced gradient approximation at each iteration. This leads to a significant reduction in cost. Numerical experiments from finance and engineering illustrate the performance and efficacy of the presented algorithms.

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MS44

Accelerating Stochastic Optimization of Separable Deep Neural Networks via Iterative Sampling Methods

Deep neural networks (DNNs) are versatile machine learning tools, but can be difficult to train to sufficient accuracy with first-order methods. In this talk, we accelerate training by exploiting the separability of most DNN architectures; that is, we separate the DNN into a nonlinear feature extractor followed by a linear model. We use the fact that the weights of the linear model can be obtained using convex optimization, which reduces the training problem. However, this has a proclivity to overfit, and hence requires training on sufficiently large samples of data. This can be prohibitively expensive storage-wise, particularly on GPUs. To overcome this limitation and the expensive task of hyperparameter tuning, we use an iterative sampled limited-memory Tikhonov method, a memory-efficient stochastic approximation approach with automatic regularization parameter tuning. We show that our method can train DNNs to high accuracy with minimal computational overhead through several numerical experiments.

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MS44

Sketchy Empirical Natural Gradient Methods for Deep Learning

We develop an efficient sketchy empirical natural gradient method (SENG) for large-scale deep learning problems. The empirical Fisher information matrix is usually low-rank since the sampling is only practical on a small amount of data at each iteration. Although the corresponding natural gradient direction lies in a small subspace, both the computational cost and memory requirement are still not tractable due to the high dimensionality. We design randomized techniques for different neural network structures to resolve these challenges. For layers with a reasonable dimension, sketching can be performed on a regularized least squares subproblem. Otherwise, since the gradient is a vectorization of the product between two matrices, we apply sketching on the low-rank approximation of these matrices to compute the most expensive parts. A distributed version of SENG is also developed for extremely large-scale applications. Global convergence to stationary points is established under some mild assumptions and a fast linear convergence is analyzed under the neural tangent kernel (NTK) case. Extensive experiments on convolutional neural networks show the competitiveness of SENG compared with the state-of-the-art methods. On the MLPerf base task ResNet-50 with ImageNet-1k, SENG achieves 75.9% Top-1 testing accuracy within 41 epochs.

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MS45

Exploiting Constant Trace Property in Polynomial Optimization

We prove that every semidefinite moment relaxation of a polynomial optimization problem (POP) with a ball constraint can be reformulated as a semidefinite program involving a matrix with constant trace property (CTP). As a result such moment relaxations can be solved efficiently by first-order methods that exploit CTP, eg, the conditional gradient-based augmented Lagrangian method. We also extend this CTP-exploiting framework to large-scale POPs with different sparsity structures. The efficiency and scalability of our framework are illustrated on second-order moment relaxations for various randomly generated quadratically constrained quadratic programs. Based on joint works with Jean-Bernard Lasserre, Victor Magron and Jie Wang.

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MS45

Local Hyperbolic Relaxations of Hyperbolic Programs

Hyperbolic programming is the problem of minimizing a linear function over the hyperbolicity cone of a hyperbolic polynomial, a special case of convex programming with a strong algebraic structure. It generalises semidefinite programming, although it is still an open question whether such generalization is strict. I will review the basic algebraic theory of hyperbolic polynomials and hyperbolic programming, and I will mention a work in progress concerning hyperbolic relaxations. I will highlight the the special case of hyperbolic relaxations of linear programming.

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MS45

High Performance Solver for Binary Pop Problems

We present BiqBin, an exact solver for linearly constrained binary quadratic problems. Our approach is based on an exact penalty method to first efficiently transform the original problem into an instance of Max-Cut, and then to solve the Max-Cut problem by a branch-and-bound algorithm. All the main ingredients are carefully developed using new semidefinite programming relaxations obtained by strengthening the existing relaxations with a set of hypermetric inequalities, applying the bundle method as the bounding routine and using new strategies for exploring the branch-and-bound tree. Furthermore, an efficient C implementation of a sequential and a parallel branch-and-bound algorithm is presented. The latter is based on a load coordinator-worker scheme using MPI for multi-node parallelization and is evaluated on a high-performance computer. The new solver is benchmarked against BiqCrunch, GUROBI, and SCIP on four families of (linearly constrained) binary quadratic problems. Numerical results demonstrate that BiqBin is a highly competitive solver. The serial version outperforms the other three solvers on the majority of the benchmark instances. We also evaluate the parallel solver and show that it has good scaling properties. The general audience can use it as an on-line service available at `http://www.biqbin.eu`.

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MS45

Exploiting Sparsity in Polynomial Optimization

Over the past twenty years, the moment-SOS hierarchy has become a powerful tool to handle polynomial optimization and possesses nice theoretical properties. From the view of applications, the bottleneck of the moment-SOS hierarchy is that the involved sequence of SDP relaxations becomes intractable very quickly as the problem size increases. In this talk, I will show how to exploit various sparsity patterns hidden in the problem data to develop sparsity-adapted moment-SOS hierarchies. As a consequence, we are able to solve practical polynomial optimization problems involving up to several thousand variables and constraints.

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MS46

Robust Phase Retrieval with Sparse Noise

We extend the Candes-Tao theory for recovering solutions to the compressed sensing problem with sparse errors via ℓ_1 regression to the real phase retrieval problem. The analysis depends on a key new property of the coding matrix called the *Absolute Range Property* (ARP) which is the analogue to the Null Space Property (NSP) in compressed sensing. When the residuals are computed using squared magnitudes, the ARP follows from a standard Restricted Isometry Property (RIP). However, when the residuals are computed using absolute magnitudes, a different kind of RIP or growth property is required. After presenting our main recovery results we describe some new iteratively reweighted algorithms for phase retrieval and their numerical performance.

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MS46

Stochastic Algorithms with Geometric Step Decay Converge Linearly on Sharp Functions

Stochastic (sub)gradient methods require step size schedule tuning to perform well in practice. Classical tuning strategies decay the step size polynomially and lead to optimal sublinear rates on (strongly) convex problems. An alternative schedule, popular in nonconvex optimization, is called *geometric step decay* and proceeds by halving the step size after every few epochs. In recent work, geometric step decay was shown to improve exponentially upon classical sublinear rates for the class of *sharp* convex functions. In this work, we ask whether geometric step decay similarly improves stochastic algorithms for the class of sharp nonconvex problems. Such losses feature in modern statistical recovery problems and lead to a new challenge not present in the convex setting: the region of convergence is local, so one must bound the probability of escape. Our main result shows that for a large class of stochastic, sharp, nonsmooth, and nonconvex problems a geometric step decay schedule endows well-known algorithms with a local linear rate of convergence to global minimizers. This guarantee applies to the stochastic projected subgradient, proximal point, and prox-linear algorithms. As an application of our main result, we analyze two statistical recovery tasks—phase retrieval and blind deconvolution—and match the best known guarantees under Gaussian measurement models and establish new guarantees under heavy-tailed distributions.

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MS47

A New Quasi-Newton Method for Minimax Problems

We introduce a novel nonsymmetric quasi-Newton step to solve the nonlinear system of equations arising from minimax problems where the Jacobian has a special block structure. Our update formula could be considered as a generalization of Powell symmetric Broyden (PSB) method to minimax problems. We show that our unit-step quasi-Newton method locally converges superlinearly. With the aid of a naive backtracking line-search we turn our nonsymmetric step into a practical algorithm and demonstrate its effectiveness on strongly convex-concave and bilinear minimax problems starting from anywhere. Our experiments show that the method maintains its local superlinear convergence property when used in conjunction with the line-search. We also use our step in a trust-region model and with additional assumptions introduce an algorithm which is globally convergent with a local R-superlinear convergence rate.

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MS47

The Landscape of Nonconvex-Nonconcave Minimax Optimization

Minimax optimization has become a central tool in machine learning with applications in robust optimization, reinforcement learning, GANs, etc. These applications are often nonconvex-nonconcave, but the existing theory is unable to identify and deal with the fundamental difficulties this poses. In this paper, we study the classic proximal point method (PPM) applied to nonconvex-nonconcave minimax problems. We develop a new analytic tool, the saddle envelope, generalizing the Moreau envelope. The saddle envelope not only smooths the objective but can convexify and concavify it based on the level of interaction present between the minimizing and maximizing variables. From this, we identify three distinct regions of nonconvex-nonconcave problems. When interaction is sufficiently strong, we derive global linear convergence guarantees. Conversely when the interaction is fairly weak, we derive local linear convergence guarantees with a proper initialization. Between these two settings, we show that PPM may diverge or converge to a limit cycle.

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MS47

Near-Optimal Algorithms for Minimax Optimization

This paper resolves a longstanding open question pertaining to the design of near-optimal first-order algorithms for smooth and strongly-convex-strongly-concave minimax problems. Current state-of-the-art first-order algorithms find an approximate Nash equilibrium using $\tilde{O}(\kappa_x + \kappa_y)$

or $\tilde{O}(\min\{\kappa_x\sqrt{\kappa_y}, \sqrt{\kappa_x}\kappa_y\})$ gradient evaluations, where κ_x and κ_y are the condition numbers for the strong-convexity and strong-concavity assumptions. A gap still remains between these results and the best existing lower bound $\tilde{\Omega}(\sqrt{\kappa_x\kappa_y})$. This paper presents the first algorithm with $\tilde{O}(\sqrt{\kappa_x\kappa_y})$ gradient complexity, matching the lower bound up to logarithmic factors. Our algorithm is designed based on an accelerated proximal point method and an accelerated solver for minimax proximal steps. It can be easily extended to the settings of strongly-convex-concave, convex-concave, nonconvex-strongly-concave, and nonconvex-concave functions. This paper also presents algorithms that match or outperform all existing methods in these settings in terms of gradient complexity, up to logarithmic factors.

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MS48

Scalable Parallel Nonlinear Optimization with PyNumero and Parapint

We present Parapint (https://github.com/parapint/parapint), an open-source Python package for efficient, scalable, parallel solution of structured nonlinear programs (NLPs). Parapint builds on Pyomo, utilizing PyNumeros interfaces to the AMPL Solver Library (ASL) for automatic differentiation (AD) and the HSL linear solver MA27 for solution of symmetric indefinite linear systems. Additionally, Parapint exploits problem structure for parallel computation on distributed memory machines with PyNumeros MPI-based matrices and vectors. Currently, Parapint contains both serial and parallel implementations of a Schur-Complement based interior-point algorithm, which can be used to solve either dynamic or stochastic optimization problems. The parallel version exploits any sparsity in the Schur-Complement to minimize communication overhead, which is critical for dynamic optimization problems. Our numerical results on a stochastic quadratic program (QP) demonstrate nearly perfect scaling to over 1,000 cores. Moreover, on a 2-dimensional partial differential equation (PDE)-constrained optimal control problem, we obtain over 360 times speedup (on 1024 cores) compared to the full-space, serial algorithm. Our results demonstrate that Parapint is a high-level framework for efficient, scalable, parallel solution of NLPs.

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MS48

An Inexact Trust-Region Newton Method for Large-Scale Convex-Constrained Optimization

We describe an inexact matrix-free trust-region algorithm for solving convex-constrained optimization problems in Hilbert space. Our algorithm uses the spectral projected gradient method to compute trial steps and is simple to implement. To project onto the intersection of the feasible set and the trust region, we reformulate and solve the dual projection problem as a one-dimensional root finding problem. We demonstrate our algorithms performance on various problems from data science and PDE-constrained topology optimization.

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MS48

Linear Systems Arising in Interior Methods for Convex Optimization: A Symmetric Formulation with Bounded Condition Number

We provide eigenvalues bounds for a new formulation of the step equations in interior methods for convex quadratic optimization. The matrix of our formulation, named K2.5, has bounded condition number, converges to a well-defined limit under strict complementarity, and has the same size as the traditional, ill-conditioned, saddle-point formulation. We evaluate the performance in the context of a Matlab object-oriented implementation of PDCO, an interior-point solver for minimizing a smooth convex function subject to linear constraints. The main benefit of our implementation, named PDCOO, is to separate the logic of the interior-point method from the formulation of the system used to compute a step at each iteration and the method used to solve the system. Thus, PDCOO allows easy addition of a new system formulation and/or solution method for experimentation. Our numerical experiments indicate that the K2.5 formulation has the same storage requirements as the traditional ill-conditioned saddle-point formulation, and its condition is often more favorable than the unsymmetric block 3x3 formulation.

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MS48

Exploiting Structure in Risk-Averse PDE-Constrained Optimization: An Interior Point Approach

PDE-constrained stochastic optimization problems provide an intuitive and potentially data-driven modeling paradigm for applications in engineering and the natural sciences. Using ideas from traditional stochastic programming, it is possible to build optimization models that yield robust optimal designs and controls. One possibility is to employ risk measures as a model of risk preference. Doing so yields risk-averse PDE-constrained optimization problems. We consider a well-known reformulation of convex combinations of the mean plus average value-at-risk as a constrained optimization problem to reformulate the risk-averse optimization problem into one with almost sure inequality constraints. This structure can be exploited by an interior point approach that leads not only to a new class of risk measures, but a competitive numerical optimization algorithm. The viability of the approach is demonstrated via numerical examples.

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MS49

Trust-Region Methods for Nonsmooth Nonconvex Problems

A Proximal Quasi-Newton Trust-Region Method for Composite Optimization We describe a trust-region method for minimizing the sum of separable nonconvex terms: a smooth term f and a nonsmooth term h. Our method minimizes a model of f + h in a trust region, which may itself be nonconvex and should coincide with f + h in value and directional derivatives at the center of the trust region. Steps are computed by a first-order method, such as the proximal gradient method or its accelerated variants. We establish global convergence to a first-order stationary point under the assumptions that f is continuously differentiable and h is proper and lower semi-continuous. We establish a complexity bound that matches the best attainable complexity bound of trust-region methods for smooth optimization. We study a special instance in which we employ a limited-memory quasi-Newton model of f, resulting in an implementation of a prox-quasi-Newton method. We describe our Julia implementation and report numerical results on inverse problems from sparse optimization and signal processing.

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MS49

Robust Least Squares for Quantized Data Matrices

Linear regression models frequently assume additive noise on dependent variables alone, i.e., Ax = b+z with z being random. In practice, the design/data matrix A is often subject to variability as well. In this talk, we draw on ideas from robust optimization and maximum likelihood estimation to formulate objectives that exploit structure in noise models with uncertainty in A. We discuss algorithms to solve the resulting nonsmooth optimization problems and compare our results to classical methods such as ordinary and total least squares. Special attention is given to the case of quantization error for applications arising in signal processing.

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MS49

Stochastic Damped L-BFGS with Controlled Norm of the Hessian Approximation

We propose a new stochastic variance-reduced damped L-BFGS algorithm, where we leverage estimates of bounds on the largest and smallest eigenvalues of the Hessian approximation to balance its quality and conditioning. Our algorithm, VARCHEN, draws from a previous work that proposed a stochastic damped L-BFGS algorithm called SdLBFGS. We establish almost sure convergence to a stationary point and a complexity bound. Moreover, we empirically demonstrate that VARCHEN is more robust than SdLBFGS-VR and SVRG on a modified DavidNet problem—a highly nonconvex and ill-conditioned problem that arises in the context of deep learning, and that their performance is comparable on a logistic regression problem and a nonconvex support-vector machine problem.

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MS49

Adaptive Proximal Stochastic Gradient Descent

We consider the training of structured neural networks where the regularizer can be non-smooth and possibly nonconvex. Such a problem arises in many applications where a sparse neural network is desirable, e.g. inferring nonlinear granger causality (Tank et al 2017, Khanna and Tan 2020). While popular machine learning libraries have adopted stochastic (adaptive) subgradient approaches, the use of proximal gradient methods in the stochastic setting has been little explored, especially with respect to the incorporation of adaptivity, which is a key ingredient in popular stochastic gradient approaches. In this talk we present a framework for stochastic proximal gradient descent that allows for arbitrary positive preconditioners. When departing from element-wise sparsity, the resulting weighted proximal maps are no longer available in closed form (in contrast to the case without preconditioning). We derive an efficient procedure to compute the prox, and consider nonconvex alternatives. We evaluate the proposed approaches on simulated and real datasets.

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MS50

Complexity, Exactness, and Rationality in Polynomial Optimization

We focus on rational solutions or nearly-feasible rational so- lutions that serve as certificates of feasibility for polynomial optimization problems. We show that, under some separability conditions, certain cubic polynomially constrained sets admit rational solutions. However, we show in other cases that it is NP Hard to detect if rational solutions exist or if they exist of any reasonable size. Lastly, we show that in fixed dimension, the feasibility problem over a set defined by polynomial inequalities is in NP.

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MS50

Proximity in Concave Integer Quadratic Programming

A classic result by Cook, Gerards, Schrijver, and Tardos provides an upper bound of $n\Delta$ on the proximity of optimal solutions of an Integer Linear Programming problem and its standard linear relaxation. In this bound, n is the number of variables and Δ denotes the maximum of the absolute values of the subdeterminants of the constraint matrix. Hochbaum and Shanthikumar, and Werman and Magagnosc showed that the same upper bound is valid if a more general convex function is minimized, instead of a linear function. No proximity result of this type is known when the objective function is nonconvex. In fact, if we minimize a concave quadratic, no upper bound can be given as a function of n and Δ. Our key observation is that, in this setting, proximity phenomena still occur, but only if we consider also approximate solutions instead of optimal solutions only. In our main result we provide upper bounds on the distance between approximate (resp., optimal) solutions to a Concave Integer Quadratic Programming problem and optimal (resp., approximate) solutions of its continuous relaxation. Our bounds are functions of n, Δ, and a parameter ϵ that controls the quality of the approximation. Furthermore, we discuss how far from optimal are our proximity bounds.

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MS50

Constructing Lattice-Free Gradient Polyhedra in Dimension Two

Lattice-free gradient polyhedra can be used to certify optimality for mixed-integer convex minimization models. We consider how to construct these polyhedra for unconstrained models with two integer variables under the assumption that all level sets are bounded. In this setting, a classic result of Bell, Doignon, and Scarf states the existence of a lattice-free gradient polyhedron with at most four facets. We present an algorithm for creating a sequence of gradient polyhedra, each of which has at most four facets, that finitely converges to a lattice-free gradient polyhedron. Each update requires constantly many gradient evaluations. Our updates imitate the gradient descent algorithm, and consequently, it yields a gradient descent type of algorithm for problems with two integer variables.

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MS51

Overcoming Inversion Bias in Distributed Newton's Method

In distributed numerical linear algebra, we often encounter inversion bias: if we want to compute a quantity that depends on the inverse of a sum of distributed matrices, then the sum of the inverses does not equal the inverse of the sum. An example of this occurs in distributed Newton's method, where we wish to compute (or implicitly work with) the inverse Hessian multiplied by the gradient. In this case, local estimates computed based on a uniform sample of data are biased, and so taking a simple average will not recover the correct solution. In this talk, I will present several methods for overcoming inversion bias. The first approach, called determinantal averaging, reweighs the biased local estimates of the Newton step before averaging them, which corrects the bias of the global estimate. Next, I will introduce a family of randomized methods for constructing small sketches of data, called surrogate sketching. These sketches use non-uniform sampling to correct the inversion bias in the Newton estimates, which makes simple averaging of these estimates very effective. Finally, I will demonstrate that for certain regularized optimization tasks, such as ridge regression, a simple heuristic of down-scaling the regularization parameter when computing the local estimates can drastically reduce the inversion bias. I will go over theoretical guarantees as well as practical trade-offs and empirical results for the presented methods.

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MS51

Systematic Second-Order Methods for Training, Designing, and Deploying Neural Networks

Finding the right Neural Network model and training it for a new task requires considerable expertise and extensive computational resources. Moreover, the process often includes ad-hoc rules that do not generalize to different application domains. These issues have limited the applicability and usefulness of DNN models, especially for new learning tasks. This problem is becoming more acute, as datasets and models grow larger, which increases training time, making random/brute force search approaches quickly untenable. In large part, this situation is due to the first-order stochastic gradient descent (SGD) methods that are widely used for training DNNs. Despite SGDs well-known benefits, vanilla SGD tends to perform poorly, and thus one introduces many (essentially ad-hoc) knobs and hyper-parameters to make it work. Many of these problems can be alleviated through second-order methods. In this talk, we will discuss the latest developments for using second-order methods for training, designing, and deploying Neural Network models.

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MS51

Convergence of Newton-Mr under Inexact Hessian Information

Recently, stability of Newton-CG under Hessian perturbations, i.e., inexact curvature information, have been extensively studied. Such stability analysis has subsequently been leveraged in designing variants of Newton-CG in which, to reduce the computational costs involving the Hessian matrix, the curvature is suitably approximated. Here, we do that for Newton-MR, which extends Newton-CG in the same manner that MINRES extends CG, but can be applied beyond the traditional convex settings, to invex problems. Unlike the stability analysis of Newton-CG, which relies on spectrum preserving perturbations in the sense of Lwner partial order, our work here draws from matrix perturbation theory to estimate the distance between the underlying exact and perturbed sub-spaces. Numerical experiments demonstrate great degree of stability for Newton-MR, mounting to a highly efficient algorithm in large-scale problems.

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MS51

Efficient Newton Methods for Robust Stochastic Nonconvex Optimization

First order stochastic optimizers have gained great popularity in recent years due to the growing importance of neural network training to modern computational frameworks. These methods are practically useful due to their per-iteration computational economy, but require extensive hyperparameter tuning for their applicability to specific problems. Higher order (Newton) methods can reduce the need for hyperparameters and improve per iteration convergence, but have fallen out of favor due to the nominal costs of forming and factorizing Hessians for high dimensional optimization problems. In this talk, we explore how low dimensional geometric information for Hessians arising in stochastic nonconvex optimization problems can be used to design matrix-free Newton methods that have similar per-iteration computational complexity to first order methods. These methods can reduce the dependence on hyperparameters and improve convergence. Further these methods can be adapted to guard against overfitting by using the Hessian to detect noise dominated geometric information of the stochastic energy landscape.

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MS52

Classical Symmetries and QAOA

We study the relationship between the Quantum Approximate Optimization Algorithm (QAOA) and the underlying symmetries of the objective function to be optimized. Our approach formalizes the connection between quantum symmetry properties of the QAOA dynamics and the group of classical symmetries of the objective function. The connection is general and includes but is not limited to problems defined on graphs. We show a series of results exploring the connection and highlight examples of hard problem classes where a nontrivial symmetry subgroup can be obtained efficiently. In particular we show how classical objective function symmetries lead to invariant measurement outcome probabilities across states connected by such symmetries, independent of the choice of algorithm parameters or number of layers. To illustrate the power of the developed connection, we apply machine learning techniques towards predicting QAOA performance based on symmetry considerations. We provide numerical evidence that a small set of graph symmetry properties suffices to predict the minimum QAOA depth required to achieve a target approximation ratio on the MaxCut problem, in a practically important setting where QAOA parameter schedules are constrained to be linear and hence easier to optimize.

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MS52

Performance Guarantees of MaxCut QAOA for P¿1

This talk will detail findings on performance guarantees for bounded p QAOA solving MAXCUT on 3-regular graphs. Previous work by Farhi et al. obtained a lower bound on the approximation ratio of 0.692 for p= 1. We find, by combinatorial proof, a lower bound on the approximation ratio of 0.7559 for p= 2, where worst-case graphs are those with no cycles ≤ 5. The bound holds for any graph evaluated at particular fixed angles optimal to the tree subgraph. This leads to a numerically consistent conjecture that these performance guarantees hold for all p: worst-case graphs have no cycles$\leq 2p+1$, and graphs evaluated at particular fixed angles optimal to the Bethe lattice exceed the level p performance guarantee. This conjecture implies that for 3 regular graphs, the classical angle optimization step of the QAOA may be replaced with an evaluation at a fixed set of angles, consistent with the phenomena of concentration.

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MS52

Adapt-QAOA: An Adaptive Variational Quantum Optimization Algorithm

The performance of variational quantum algorithms critically depends on the form of the ansatz. A good ansatz translates to relatively shallow circuits and involves a low number of classical optimization parameters. These features can be achieved more easily if the ansatz knows something about the problem that is simulated. In this talk, I will present our techniques for problem-tailored ansatze, including our newly developed ADAPT-QAOA for optimization problems. Our simulations show that these techniques can outperform competing ansatze in terms of CNOT count and accuracy.

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MS53

A Fast Stochastic Algorithm for Regularized PET Reconstruction

While smooth and non-smooth regularization are known to improve the quality of PET reconstruction, designing algorithms performing this task in a time compatible with the clinical standard is currently challenging. We present an algorithm which builds on the renowned Primal-Dual Hybrid Gradient (PDHG) algorithm, also known as Chambolle-Pock algorithm for convex optimization, with the added feature that it can randomly update partial variables. In the framework of PET imaging, the Stochastic Primal-Dual Hybrid Gradient (SPDHG) algorithm is able to reconstruct images from sinograms with non-smooth priors like Total Variation, which promotes sharp boundaries. The algorithm proceeds by using only a randomly chosen subset of all views at a given iteration, hence using only partial forward and back-projections, which makes it much faster than PDHG. Furthermore, SPDHG converges almost surely under a similar step-size conditions than PDHG. We illustrate this on a variety of real patient datasets from Siemens and GE scanners.

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MS53

Fast Algorithms for Initial Value Control Problems

We present fast numerical algorithms for optimal control problems with initial value control. Our contributions are the design of efficient computational methods for numerical optimization, their analysis, and their application to real-world problems. The inverse problem we are considering is commonly referred to as diffeomorphic image registration. In our formulation, we seek to find an initial momentum, which represents the initial state of a differential equation in the group of diffeomorphisms. This diffeomorphism establishes a pointwise correspondence between two images of the same object or scene, e.g., acquired at two different timepoints (the input data to our problem). We will showcase results for applications in medical imaging sciences. We will consider different formulations for this problem, and discuss the rate of convergence, accuracy, time-to-solution, and inversion quality of our formulations.

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MS53

Image-Based Modeling of Tumor Growth in Patients with Glioma

The image-based modeling of tumor growth in patient with glioma serves the purpose of improving patient diagnostics, as well as treatment. We will present a Bayesian model linking a Fisher-Kolmogorov type of tumor growth model to the information from multimodal images of the patient's tumor. We will demonstrate how to use the patient-adapted model for improving radio-therapy. Moreover, we will present extensions of the model that accelerate Bayesian parameter estimation, as well as the related forward simulation in patient-specific modeling domains, using neural networks.

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MS54

Understanding Tradeoffs in Objectives through Optimization

We attempt to understand the tradeoff between metrics for compactness and black voting-age population (BVAP) and how this varies in each state depending on their geography and demographics. We focus on the Polsby Popper objective and a modified objective accounting for the probability of election of a black representative based on the ratio of the black voting-age population and voting-age population in a district. These are both highly non-convex objective functions that are difficult to deal with. We generate many solutions using heuristics based on the recombination MCMC methods of the MGGG group. We present improvements on these heuristics, motivating theory, and some integer programming models.

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MS56

Stochastic First-order Methods for Saddle-point Problems Under Differential Privacy Constraint

In this talk, we present the first systematic study of stochastic variational inequality (SVI) and stochastic saddle point (SSP) problems under the constraint of differential privacy-(DP). We propose two algorithms: Noisy Stochastic Extragradient (NSEG) and Noisy Inexact Stochastic Proximal Point (NISPP) which can be applied to both SVI and SSP problems. We show that sampling with replacement variants of these algorithms attain the optimal risk for DP-SVI and DP-SSP. Key to our analysis is the investigation of algorithmic stability bounds, both of which are new even in the nonprivate case, together with a novel stability implies generalization result for the gap functions for SVI and SSP problems. The dependence of the running time of NSEG method, with respect to the dataset size n, is n^2. This runtime can be accelerated to $\tilde{O}(n^{3/2})$ for NISPP by showing stronger stability guarantess.

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MS56

An Accelerated Inexact Proximal Point Method for Solving Nonconvex-Concave Min-Max Problems

This talk presents a quadratic-penalty type method for solving unconstrained and linearly-constrained composite nonconvex-concave min-max problems. The method for both cases consists of solving a sequence of proximal subproblems which, due to the min-max structure of the problem, are potentially nonsmooth but can be approximated by smooth composite nonconvex minimization problems. Each of these proximal subproblems is then solved by applying an accelerated method to its corresponding smooth composite nonconvex approximation. Iteration complexity bounds for obtaining approximate stationary points of both cases are also established. Finally, numerical results are given to demonstrate the efficiency of the proposed unconstrained method.

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MS56

A Proximal Bundle Variant with Optimal Iteration-Complexity for a Large Range of Prox Stepsizes

This talk presents a proximal bundle variant, namely, the relaxed proximal bundle (RPB) method, for solving convex nonsmooth composite optimization problems. Like other proximal bundle variants, RPB solves a sequence of prox bundle subproblems whose objective functions are regularized composite cutting-plane models. Moreover, RPB uses a novel condition to decide whether to perform a serious or null iteration which does not necessarily yield a function value decrease. Optimal iteration-complexity bounds for RPB are established for a large range of prox stepsizes, both in the convex and strongly convex settings. To the best of our knowledge, this is the first time that a proximal bundle variant is shown to be optimal for a large range of prox stepsizes. Finally, iteration-complexity results for RPB to obtain iterates satisfying practical termination criteria, rather than near optimal solutions, are also derived.

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MS56

Complexity of Proximal Augmented Lagrangian Type Methods for Solving Nonconvex Linearly Constrained Composite Optimization Problems

This talk presents the iteration-complexity of an inner accelerated inexact proximal augmented Lagrangian (IAPIAL) method for solving linearly constrained smooth nonconvex composite optimization problems which is based on the classical Lagrangian function and, most importantly, performs a full Lagrangian multiplier update, i.e., no shrinking factor is incorporated on it. More specifically, each IAPIAL iteration consists of inexactly solving a proximal augmented Lagrangian subproblem by an accelerated composite gradient (ACG) method followed by a full Lagrange multiplier update. Under the assumption that the domain of the composite function is bounded and the problem has a Slater point, it is shown that IAPIAL generates an approximate stationary solution in at most $\mathcal{O}(\log(1/\rho)/\rho^3)$ ACG iterations, where $\rho > 0$ is the tolerance for both stationarity and feasibility. Finally, the above bound is derived without assuming that the initial point is feasible.

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MS57

Solving Composite Fixed Point Problems with Block Updates

Various strategies are available to construct iteratively a common fixed point of nonexpansive operators by activating only a block of operators at each iteration. In the more challenging class of composite fixed point problems involving operators that do not share common fixed points, current methods require the activation of all the operators at each iteration, and the question of maintaining convergence while updating only blocks of operators is open. We propose a method that achieves this goal and analyze its asymptotic behavior. Weak, strong, and linear convergence results are established by exploiting a connection with the theory of concentrating arrays. Applications to several nonlinear and nonsmooth analysis problems are presented, ranging from monotone inclusions and inconsistent feasibility problems, to variational inequalities and minimization problems arising in data science.

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MS57

Projection Methods for Neural Network Training: A Nonconvex Inconsistent Set Feasibility Framework

In this talk, we demonstrate a procedure to find projection onto hyperbola and hyperboloid sets in Hilbert spaces. These sets are crucial in many learning applications, according to Elser's recently proposed framework. We also explore the framework's adaptability using an example of neural network training with projection methods.

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MS57

The Bregman Proximal Average

We propose a proximal average in the framework of Bregman distances.

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MS58

Reduced Order Methods and Shape Optimisation: State of the Art and Perspectives from Industry to Medicine

We focus on non-intrusive model order reduction in computational fluid dynamics to allow efficient iterative shape optimisation processes in parametric domains. We deal with parameter space reduction, properly integrated in our

reduced computational pipeline. Computational reduction developments deal with turbulence modelling thanks to a data-driven hybrid approach. Geometrical parametrisation is based on free form deformation. Examples of applications are taken from naval engineering, for example a shape optimisation process of a cruise ship hull, and from biomedical engineering in cardiovascular problems.

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MS58

Higher Order and Non-Smooth Optimization of Shells with Applications in 3D Imaging and Micro Fluids

Efficient optimization schemes for shape optimization of shells are presented. One the one hand, these arise when the geometry is driven by geometric flows and such problems appear naturally when regularizing inverse problems. On the other hand, they also appear in applications such as micro-fluids when the shape of bubbles and capillary bridges are interpreted as optimal solutions of the Young-Laplace Problem. To this end, we consider both a Newton-Scheme for computing capillary bridges and droplets via total energy minimization subject to wetting constraints as well as non-smooth algorithms when the geometric flow stems from, e.g., the total (generalized) variation of the normal.

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MS58

Nonlinear Self-Adapting Shape Metrics in Aerodynamic Optimization

In this talk we present algorithmic approaches for shape optimization problems requiring large and robust deformations. Typical applications include processes described by PDEs where there is only a small number of materials or parameters to be identified by the contour of their distribution. Here we consider shape optimization problems as optimal control problems via the method of mappings. Thus, instead of optimizing over a set of admissible shapes, the problem is reformulated as optimization in a set of admissible transformations to a reference shape. Taking this continuous perspective on the shape optimization problem leads to versatile algorithmic optimization approaches. The focus of our presentation is on the choice of nonlinear extension models linking the boundary control to a field deformation. We demonstrate how these extensions can be adapted to the underlying problem. This allows to require properties like local injectivity of transformations and retain mesh quality even under large deformations. The results are substantiated with numerical examples in optimal aerodynamic design.

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MS58

Topology Optimisation on Surfaces via the Topological Derivative

In this task we discuss the problem of the optimal distribution of two materials on smooth submanifolds M of dimension $d-1$ in R^d without boundary by means of the topological derivative. We consider a class of shape optimisation problems which are constrained by a linear partial differential equation on the surface. We examine the singular perturbation of the differential operator and material coefficients and derive the topological derivative. Finally, we show how the topological derivative in conjunction with a level set method on the surface can be used to solve the topology optimisation problem numerically.

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MS59

Non-Convexity from Symmetry: the Viewpoint of Lifts to Manifolds

Certain optimization problems are non-convex in a way that can be attributed directly to symmetries. Think for example of a smooth cost function having two distinct global optima: it is easy to imagine how their presence can lead to the existence of saddle points. I will discuss such problems from the perspective of smooth lifts (maps from a smooth manifold onto a domain, and whose fibers capture the symmetries of the problem). Studying these lifts informs us about whether and how the symmetric landscape inherits possibly favorable properties of the landscape where symmetries have been removed. This is particularly relevant when it is more convenient to run optimization algorithms on the symmetric landscape. Joint work with Eitan Levin (CalTech) and Joe Kileel (UT Austin).

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MS59

Decentralized Riemannian Gradient Descent on the Stiefel Manifold

In this talk, we consider a distributed non-convex optimization where a network of agents aims at minimizing a global function over the Stiefel manifold. The global function is represented as a finite sum of smooth local functions, where each local function is associated with one agent and agents communicate with each other over an undirected connected graph. The problem is non-convex as local functions are possibly non-convex (but smooth) and the Steifel manifold is a non-convex set. We first establish the Q-linear rate of Riemannian consensus on Stiefel manifold in a local consensus region. Then, we present a decentralized Riemannian stochastic gradient method (DRSGD) with the convergence rate of $\mathcal{O}(1/\sqrt{K})$ to a stationary point. To have exact convergence with constant stepsize, we also propose a decentralized Riemannian gradient tracking algorithm (DRGTA) with the convergence rate of $\mathcal{O}(1/K)$ to a stationary point. We use multi-step consensus to preserve the iteration in the local (consensus) region. DRGTA is the first decentralized algorithm with exact convergence for distributed optimization on Stiefel manifold.

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MS59

Riemannian Optimization on the Symplectic Stiefel Manifold

The symplectic Stiefel manifold, denoted by Sp(2p,2n), is the set of linear symplectic maps between the standard symplectic spaces Sp(2p) and Sp(2n). When p=n, it reduces to the well-known set of 2n-by-2n symplectic matrices. Optimization problems on Sp(2p,2n) find applications in various areas, such as optics, quantum physics, numerical linear algebra and model order reduction of dynamical systems. In this talk, we propose and analyze gradient-descent methods on Sp(2p,2n), where the notion of gradient stems from a Riemannian metric. We consider a novel Riemannian metric on Sp(2p,2n) akin to the canonical metric of the (standard) Stiefel manifold. In order to perform a feasible step along the antigradient, we develop two types of search strategies: one is based on quasi-geodesic curves, and the other one on the symplectic Cayley transform. The resulting optimization algorithms are proved to converge globally to critical points of the objective function. Numerical experiments illustrate the efficiency of the proposed methods. This is a joint work with Nguyen Thanh Son, P.-A. Absil and Tatjana Stykel.

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MS59

A Riemannian Block Coordinate Descent Method for Computing the Projection Robust Wasserstein Distance

The Wasserstein distance has become increasingly important in machine learning and deep learning. Despite its popularity, the Wasserstein distance is hard to approximate because of the curse of dimensionality. A recently proposed approach to alleviate the curse of dimensionality is to project the sampled data from the high dimensional probability distribution onto a lower-dimensional subspace, and then compute the Wasserstein distance between the projected data. However, this approach requires to solve a max-min problem over the Stiefel manifold, which is very challenging in practice. The only existing work that solves this problem directly is the RGAS (Riemannian Gradient Ascent with Sinkhorn Iteration) algorithm, which requires to solve an entropy-regularized optimal transport problem in each iteration, and thus can be costly for large-scale problems. In this paper, we propose a Riemannian block coordinate descent (RBCD) method to solve this problem, which is based on a novel reformulation of the regularized max-min problem over the Stiefel manifold. We show that the complexity of arithmetic operations for RBCD to obtain an ϵ-stationary point is $O(\epsilon^{-3})$. This significantly improves the corresponding complexity of RGAS, which is $O(\epsilon^{-12})$. Moreover, our RBCD has very low per-iteration complexity, and hence is suitable for large-scale problems.

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MS60

Estimation of Sparse Gaussian Graphical Models with Hidden Clustering Structure

Estimation of Gaussian graphical models is important in natural science when modeling the statistical relationships between variables in the form of a graph. The sparsity and clustering structure of the concentration matrix is enforced to reduce model complexity and describe inherent regularities. We propose a model to estimate the sparse Gaussian graphical models with hidden clustering structure, which also allows additional linear constraints to be imposed on the concentration matrix. We design an efficient two-phase algorithm for solving the proposed model. We develop a symmetric Gauss-Seidel based alternating direction method of multipliers (sGS-ADMM) to generate an initial point to warm-start the second phase algorithm, which is a proximal augmented Lagrangian method (pALM), to get a solution with high accuracy. Numerical experiments on both synthetic data and real data demonstrate the good performance of our model, as well as the efficiency and robustness of our proposed algorithm.

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MS60

A Note on Variational Analysis of Nonsmooth Composite Matrix Optimization Problem

Nonsmooth composite matrix optimization problem(CMatOP) is a generalization of the matrix conic programming problem with wide applications in numerical linear algebra, computational statistics and engineering. Many well known problems like SDP, eigenvalue minimization and matrix completion are a special case of it. We study several variational properties of a class of non-polyhedral functions and characterize the limiting normal cone of it. Based on it, we also give the characterization of Lipschitz full stability of CMatOP and study its relationship with strong regularity and strong second order sufficient condition.

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MS61

Bounding Optimality Gaps via Bagging

We study a statistical method to estimate the optimality gap of a given solution for stochastic optimization as an assessment of the solution quality. Our approach is based on bootstrap aggregating, or bagging, resampled sample average approximation (SAA). We show how this approach leads to valid statistical confidence bounds for non-smooth optimization, and demonstrate its statistical strengths and stability compared to existing methods. We also present our theory that views SAA as a kernel in an infinite-order symmetric statistic, which leads to some generalizations of classical central limit results for SAA.

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MS61

Retrospective Approximation for Nonsmooth Convex Stochastic Optimization

We consider nonsmooth convex stochastic optimization problems with a first-order stochastic oracle over decision variables that live in normed space. We present an iterative algorithm where a "practical" solver such as the level method can be invoked repeatedly to solve a sequence of deterministic problems and generate stochastic iterates having optimality gaps that converge (almost surely and in L-1) to zero. Apart from the standard results on iteration and work complexity, we demonstrate a central-limit theorem leading to an inference result that can be used for exact confidence interval construction and optimal stopping.

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MS61

Variance-Reduced Accelerated First-Order Methods: Central Limit Theorems and Confidence Statements

In this paper, we study a stochastic strongly convex optimization prob- lem and propose three classes of variable sample-size stochastic first-order methods including the standard stochastic gradient descent method, its accelerated variant, and the stochastic heavy ball method. In the iterates of each scheme, the unavail- able exact gradients are approximated by averaging across an increasing batch size of sampled gradients. We prove that when the sample-size increases geomet- rically, the generated estimates converge in mean to the optimal solution at a geometric rate. Based on this result, we provide a unified framework to show that the rescaled estimation errors converge in distribution to a normal distribution, in which the covariance matrix depends on the Hessian matrix, covariance of the gradient noise, and the steplength. If the sample-size increases at a polynomial rate, we show that the estimation errors decay at the corresponding polynomial rate and establish the corresponding central limit theorems (CLTs). Finally, we provide an avenue to construct confidence regions for the optimal solution based on the established CLTs, and test the theoretical findings on a stochastic parameter estimation problem.

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MS61

Data-Driven Compositional Optimization in Misspecified Regimes

As systems grow in size, scale, and intricacy, the challenges of misspecification become even more pronounced. In this paper, we focus on parametric misspecification in regimes complicated by risk and nonconvexity. When this misspecification may be resolved via a parallel learning process, we develop data-driven schemes for resolving a broad class of misspecified stochastic compositional optimization problems. Notably, this rather broad class of compositional problems can contend with challenges posed by diverse forms of risk, dynamics, and nonconvexity, significantly extending the reach of such avenues. Specifically, we consider the minimization of a stochastic compositional function $\mathbb{E}[f(\mathbb{E}[g(x;\theta_2^*,\xi_2)];\theta_1^*,\xi_1)]$ over a closed and convex set $\mathcal{X}$ in a regime where parameters θ_1^* and θ_2^* are unknown, and ξ_1 and ξ_2 are two suitably defined random variables. Existing algorithms can accommodate settings where parameters θ_1^* and θ_2^* are known, but efficient first-order schemes are hitherto unavailable for the imperfect information compositional counterparts. Via a data-driven compositional optimization (DDCO) approach, we develop asymptotic and rate guarantees for unaccelerated and accelerated schemes for convex, strongly convex, and nonconvex problems in a two-level regime. Additionally, we extend the accelerated schemes to the general T-level setting. Notably, the non-asymptotic rate guarantees in all instances show no degradation from the rate statements obtained in a correctly specified regime. Our numerical experiments support the theoretical findings based on the resolution of a three-level compositional risk-averse optimization problem.

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MS62

A Game Theoretic Perspective on Bayesian Multi-Objective Optimization

We address the question how to efficiently solve many-objective optimization problems, in a computationally demanding or black-box simulation context?. We shall motivate the question by applications in machine learning and engineering, and discuss specific harsh challenges in using classical Pareto approaches when the number of objectives is four or more. Then, we review solutions combining approaches from Bayesian optimization,e.g., with Gaussian processes, and concepts from game theory like Nash equilibria, Kalai-Smorodinsky solutions and detail extensions like Nash-Kalai-Smorodinsky solutions. We finally introduce the corresponding algorithms and provide some illustrating results.

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MS62

PDE-Constrained Games and Some Emerging Applications

Differential games involve state equations governed by system of differential equations. They model a huge variety of competitive interactions, in social behavior, economics, biology among many others, predator-prey, pursuit-evasion games and so on. Engineering applications are rather rare and quite new. We shall present a non exhaustive overview of newly developed engineering (in a large sense) applications, and shall pay a specific attention to applications in inverse problems, and notably in what we call multi-inverse problems. In the latter new framework, game theory turns up to be able to setup coupled broblems that would be delicate to model with classical approaches. We shall illustrate our claims with multi-inverse problem formulations for the linear and non-linear Stokes flows, where recovery of boundary data is led jointly to shape reconstruction of obstacles or inclusions, or to pointwise source detection.

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MS62

Finite and Infinite Dimensional Extensions of Standard Nash Games

In this talk we present finite and infinite dimensional extensions of standard Nash games. First, we consider the case when the game includes a hierarchical structure, e.g. the players are divided into two groups, namely the leaders and the followers, according to their position in the game. In particular, we consider the case, where the leaders' and/or the followers' game can be described as a potential game. Another extensions considers a dynamic Stackelberg game, where the number of followers becomes very (infinitely) large. Finally, we present Nash equilibrium for a dynamic boundary control game with a star-shaped network of strings, where each string is governed by the wave equation.

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MS63

Achieving Consistency with Cutting Planes

The primary role of cutting planes is to separate fractional solutions of the linear programming relaxation, which results in tighter bounds for pruning the search tree and reducing its size. Bounding, however, has an *indirect* impact on the size of the search tree. Cutting planes can also reduce backtracking by excluding inconsistent partial assignments that occur in the course of branching, which directly reduces the tree size. The constraint programming community has studied consistency extensively and used it as an effective tool for the reduction of backtracking. We extend this approach to integer programming by defining concepts of consistency that are useful in a branch-and-bound context. We present a theoretical framework for studying these concepts, their connection with the convex hull and their power to exclude infeasible partial assignments. We introduce a new class of cutting planes that target achieving consistency rather than improving dual bounds. Computational experiments on both synthetic and benchmark instances show that the new class of cutting planes can significantly outperform classical cutting planes, such as disjunctive cuts, by reducing the size of the search tree and the solution time. More broadly, we suggest that consistency concepts offer a new perspective on integer programming that can lead to a better understanding of what makes cutting planes work when used in branch-and-bound search.

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MS63

Convexification of Constrained Nonlinear Optimization Problems with Indicator Variables

In this talk we present recent work on convexification with indicator variables. Specifically, we derive ideal convexifications for sets involving non-separable nonlinear functions, with additional constraints on both the continuous variables and indicator constraints. We show that by including and exploiting additional constraints, it is indeed possible to obtain much better convex relaxations of mixed-integer problems arising in sparse regression and portfolio optimization.

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MS63

Conic Mixed-Binary Sets: Convex Hull Characterizations and Applications

We consider a general conic mixed-binary set where each homogeneous conic constraint involves an affine function of independent continuous variables and an epigraph variable associated with a nonnegative function, f_j, of common binary variables. Sets of this form naturally arise as substructures in a number of applications including mean-risk optimization, chance-constrained problems, portfolio optimization, lot-sizing and scheduling, fractional programming, variants of the best subset selection problem, and distributionally robust chance-constrained programs. When all of the functions f_j's are submodular, we give a convex hull description of this set that relies on characterizing the epigraphs of f_j's. Our result unifies and generalizes an existing result in two important directions. First, it considers *multiple general convex cone* constraints instead of a single second-order cone type constraint. Second, it takes *arbitrary nonnegative functions* instead of a specific submodular function obtained from the square root of an affine function. We close by demonstrating the applicability of our results in the context of a number of broad problem classes.

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MS63

Quantifying Probabilities using Optimization Techniques

This paper develops techniques to estimate the probability that the optimal value of a convex program exceeds a threshold. In the process, we relate affine/polynomial policies of the robust counterpart to relaxation hierarchies in MINLP. Then, we develop counting, sampling and convexification techniques to derive the desired probability estimates. These techniques are applied to analyze the impact of link failures on network routing.

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MS64

Iteratively Reweighted Group Lasso based on Log-Composite Regularization

We introduce a new formulation and an iterative algorithm for a group-sparse representation problem where subsets of model variables form non-overlapping groups. The proposed algorithm solves a reweighted group lasso at each iteration, and computes a directional stationary solution which achieves global optimality under some conditions. We present results of numerical experiments conducted with synthetic and real datasets showing that our method achieves superior performance compared existing methods in many criteria including prediction accuracy, relative error, and group recovery success rate.

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MS64

Efficient Batch Policy Learning in Markov Decision Processes

In this talk, I will discuss the batch (off-line) reinforcement learning problem in infinite horizon Markov Decision Processes. Motivated by mobile health applications, we focus on learning a policy that maximizes the long-term average reward. Given limited pre-collected data, we propose a doubly robust estimator for the average reward and show that it achieves statistical efficiency bound. We then develop an optimization algorithm to compute the optimal policy in a parametrized stochastic policy class. The performance of the estimated policy is measured by the difference between the optimal average reward in the policy class and the average reward of the estimated policy. Under some technical conditions, we establish a strong finite-sample regret guarantee in terms of total decision points, demonstrating that our proposed method can efficiently break the curse of horizon. The performance of the proposed method is illustrated by simulation studies.

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MS65

The Newton-Bracketing Method for Solving Quadratic and Polynomial Optimization Problems

For the Lagrangian-DNN relaxation of quadratic optimization problems (QOPs), we propose a Newton-bracketing method to improve the performance of the bisection-projection method implemented in BBCPOP [ACM Tran. Softw., 2019]. The relaxation problem is converted into the problem of finding the largest zero y^* of a continuously differentiable (except at y^*) convex function $g : R \to R$ such that $g(y) = 0$ if $y \leq y^*$ and $g(y) > 0$ otherwise. In theory, the method generates lower and upper bounds of y^* both converging to y^*. Their convergence is quadratic if the right derivative of g at y^* is positive. Accurate computation of $g'(y)$ is necessary for the robustness of the method, but it is difficult to achieve in practice. As an alternative, we present a secant-bracketing method. We demonstrate that the method improves the quality of the lower bounds obtained by BBCPOP and SDPNAL+ for binary QOP instances from BIQMAC. Moreover, new lower bounds for the unknown optimal values of large scale QAP instances from QAPLIB are reported.

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MS65

Completely Positive Factorization via Orthogonality Constrained Problem

A real symmetric matrix A is completely positive if there is an entrywise nonnegative matrix B such that $A = BB^T$. Such B is called a CP factorization. The set CP_n consisting of all n by n completely positive matrices is called the completely positive cone. It has been known for two decades that many NP-hard optimizations can reduce to the minimization of a linear function over the completely positive cone. However, many fundamental open problems have been left around the completely positive cone. This manuscript is devoted to one of the open problems, which is to find a CP factorization of a completely positive matrix. We propose a new numerical method, which stems from the idea presented by Groetzner and Dr in 2020, wherein the CP factorization problem can be reformulated as a nonconvex feasibility problem. We begin to solve this feasibility problem through the use of curvilinear search method, proposed by Wen and Yin in 2013, which is designed for general orthogonality constrained problem. To apply this method, we employ a smooth approximation named LogSumExp instead of the maximum function. The numerical experiments show that our method is much faster than most of the other CP factorization algorithms. It also is reliable for most completely positive matrices.

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MS65

Error Bounds for Conic Problems and an Application to the Exponential Cone

In this talk, we propose a framework for obtaining error bounds for conic linear feasibility problems using as few assumptions as possible. Our tools include facial reduction, facial residual functions and a generalization of the notion of amenable cones. As an application, we will prove tight error bounds for conic feasibility problems over the exponential cone. Curiously, some of these tight bounds are not Hlderian and feature the logarithm function or the Boltzmann-Shannon entropy function. This is a joint work with Scott B. Lindstrom and Ting Kei Pong. More details can be seen on arxiv:2010.16391.

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MS65

A Primal-Dual Interior Point Method for Nonlinear Semi-Definite Optimization Problems using the Family of Monteiro-Tsuchiya Directions

The recent advance of algorithms for nonlinear semidefinite optimization problems, abbreviated as NSDPs, is remarkable. Yamashita et al. first proposed a primal-dual interior point method (PDIPM) for solving NSDPs using the family of Monteiro-Zhang (MZ) search directions. Since then, various kinds of PDIPMs have been proposed for NSDPs, but, as far as we know, all of them are based on the MZ family. In this talk, we present a PDIPM equipped with the family of Monteiro-Tsuchiya (MT) directions, which were originally devised for solving linear semi-definite optimization problems as were the MZ family. We further prove local superlinear convergence to a Karush-KuhnTucker point of the NSDP in the presence of certain general assumptions on scaling matrices, which are used in producing the MT scaling directions.

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MS66

DC Algorithms for a Class of Sparse Group L0 Regularized Optimization Problems

In this paper, we consider a class of sparse group L0 regularized optimization problems. Firstly, we give a continuous relaxation model of the considered problem and establish the equivalence of these two problems in the sense of global minimizers. Then, we define a class of stationary points of the relaxation problem, and prove that any defined stationary point is a local minimizer of the considered sparse group L0 regularized problem and satisfies a desirable property of its global minimizers. Further, based on the difference-of-convex (DC) structure of the relaxation problem, we design two DC algorithms to solve the relaxation problem. We prove that any accumulation point of the iterates generated by them is a stationary point of the relaxation problem. Specially, all accumulation points have a common support set and a unified lower bound for the nonzero entries, and their zero entries can be converged within finite iterations. Moreover, we prove the convergence of the entire iterates generated by the proposed algorithms. Finally, we give some numerical experiments to show the efficiency of the proposed algorithms.

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MS66

Choroid Layer Segmentation of Retinal OCT Images based on CNN Classifier and L2-Lq Fitter

Optical Coherence Tomography (OCT) is a noninvasive cross-sectional imaging technology often used to examine the retinal structure and its pathology of the eye. Evaluating the thickness of the choroid using OCT images is of great interests for clinicians and researchers to monitor the choroidal thickness in many ocular diseases for diagnosis and management. However, manual segmentation and thickness profiling of choroid are time-consuming which may lead to low efficiency in analyzing large quantity of OCT images for swift treatment of patients. In this paper, an automatic segmentation approach based on CNN classifier and $l2$-l_q $(0 < q < 1)$ fitter is presented to identify boundaries of the choroid and to generate thickness profile of the choroid from retinal OCT images. The method of detecting inner choroidal surface is motivated by its biological characteristics after light reflection, while the outer chorio-scleral interface is transferred into a classification and fitting problem. The proposed method is tested in a data set of clinically obtained retinal OCT images with ground-truth marked by clinicians. Our numerical results demonstrate the effectiveness of the proposed approach to achieve stable and accurate auto-segmentation of the choroid.

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MS66

Mini-Batch Stochastic Nesterov's Smoothing Method for Constrained Convex Stochastic Composite Optimization

This paper considers a class of constrained convex stochastic composite optimization problems whose objective function is given by the summation of a differentiable convex component, together with a nonsmooth but convex component. The nonsmooth component has an explicit max structure that may not easy to compute its proximal mapping. In order to solve these problems, we propose a mini-batch stochastic Nesterov's smoothing (MSNS) method. Convergence and the optimal iteration complexity of the method are established. Numerical results are provided to illustrate the efficiency of the proposed MSNS method for a support vector machine (SVM) model.

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MS67

Convergent Approximation of Global Minimizers of Integral Functionals

Computing a global minimizer of an integral functional $\mathcal{F}(u) = \int_\Omega f(x, u(x), \nabla u(x))\mathrm{d}x$ over all functions $u : \Omega \to \mathbb{R}^m$ constrained by boundary conditions is a fundamental challenge in many fields, including nonlinear elasticity, material science, pattern formation and analysis of partial differential equations (PDEs). This talk will revisit the decade-old idea that, when the dependence on u is polynomial, a global minimizer u^* may be approximated by discretizing $\mathcal{F}(u)$ and finding approximate discrete minimizers with sparse sum-of-squares (SOS) relaxations. I will show that if one employs well-designed finite-element (FE) discretizations and SOS relaxations with so-called chordal sparsity, then this approach is guaranteed to produce convergent approximations to u^* as the FE mesh is refined and the SOS relaxation order is raised. I will also present numerical examples demonstrating that excellent approximations to u^* are obtained in practice even when one uses computationally cheaper SOS relaxations with non-chordal sparsity, for which convergence is not guaranteed. Finally, I will briefly outline remaining theoretical and practical barriers to the extension of FE-SOS methods to PDE-constrained optimization.

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MS67

Relaxation of Variational Problems into Sum-of-Squares Programs

This talk concerns a method for bounding global optima of integral variational problems. For an integral $\int_\Omega f(x, u(x), \nabla u(x))\mathrm{d}x$, finding its global minimum, say, over all functions $u : \Omega \to \mathbb{R}^m$ that satisfy the desired integral or pointwise constraints (if any) is generally a nonconvex and intractable problem. This talk will describe methods for bounding the global minimum from below. The approach involves formulating a non-standard dual maximization problem, then relaxing this dual in a certain way to obtain a maximization problem constrained by pointwise inequalities on finite-dimensional spaces. We call the latter a pointwise dual relaxation. When the integrand f and similar functions defining the constraints are polynomials, the pointwise dual relaxation can be further relaxed into an SOS program and solved computationally, giving numerical lower bounds on the global minimum of the original variational problem. This talk will present computations of sharp lower bounds in various examples, and it will describe what is known and unknown about sharpness of the approach in general.

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MS67

Path Differentiable ODEs and Applications

This talk will be about path differentiability for dynamical systems modeled with ordinary differential equations (ODEs). Path differentiability is a regularity that has been introduced recently by J. Bolte and E. Pauwels, and which allows to define precisely some basic rules of calculus, such as the chain rule, for non-smooth objects. It allows also to characterize precisely the gradient of path differentiable vector fields and to analyze the convergence in values of some stochastic gradient descent. The work that will be presented is then an extension of this concept to a (quite large) class of dynamical systems. In this talk, it will be explained that, as soon as the vector field of the considered ODE is path differentiable, then the related flow is also path differentiable. Such a property is crucial to extend the celebrated adjoint method to the case of less regular vector fields. Our approach also allows us to compute backward and forward derivatives, which is not an easy task in general. An application to nonsmooth neural ODEs will be also presented. It is a joint work with Edouard Pauwels.

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MS67

Sparsity Exploitation in Moment-Sum-of-Squares Hierarchies for Nonlinear Dynamical Systems

We develop sparse moment-sum-of-squares approximations for three problems from nonlinear dynamical systems: region of attraction, maximum positively invariant set and global attractor. We prove general results allowing for a decomposition of these sets provided that the vector field and constraint set posses certain structure. We combine these decompositions with methods from previous works based on infinite-dimensional linear programming. For polynomial dynamics, we show that these problems admit a sparse sum-of-squares (SOS) approximation with guaranteed convergence such that the number of variables in the largest SOS multiplier is given by the dimension of the largest subsystem appearing in the decomposition. The dimension of such subsystems depends on the sparse structure of the vector field and the constraint set and can allow for a significant reduction of the size of the semidefinite program (SDP) relaxations, thereby allowing to address far larger problems without compromising convergence guarantees. The method is simple to use and based on convex optimization. Numerical examples demonstrate the approach.

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MS68

Accelerated Primal-Dual Algorithms for Distributed Smooth Convex Optimization over Networks

This paper proposes a new family of primal-dual-based distributed algorithms for smooth, convex, multi-agent optimization over networks that uses only gradient information and gossip communications. The algorithms can also employ acceleration on the computation and communications. We provide a unified analysis of their convergence rate, measured in terms of the Bregman distance associated to the saddle point reformation of the distributed optimization problem. When acceleration is employed, the rate is shown to be optimal, in the sense that it matches (under the proposed metric) existing complexity lower bounds of distributed algorithms applicable to such a class of problem and using only gradient information and gossip communications. Preliminary numerical results on distributed least-square regression problems show that the proposed algorithm compares favorably on existing distributed schemes.

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MS68

Fully Asynchronous Distributed Optimization over Directed Networks

We consider the distributed optimization problem, the goal of which is to minimize a finite sum of local objective functions over a directed network. In sharp contrast to the literature, we focus on fully asynchronous distributed methods where each node updates without waiting for any other node by using (possibly stale) information from neighbors. Thus, it is both deadlock-free and robust to any bounded communication delay. To ensure the exact convergence, we propose an aggressive mechanism to adaptively tune optimization stepsize in the sense that slow nodes dynamically increase their stepsizes to catch up fast ones. Then, we rigorously prove convergence and show their advantages over the synchronous versions, both theoretically and numerically.

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MS68

Distributed Constrained Convex Optimization over Digraphs: A Fenchel Dual Based Approach

In this talk, we consider a distributed convex optimization with local constraint sets over a strongly connected digraph, where the global objective function is described as a sum of some agentslocal objective functions. To solve the problem in a distributed way, we first resort to its Fenchel dual problem by introducing local conjugate functions. Then, we propose a distributed Fenchel dual gradient algorithm in continuous-time setting via a two-time-scale system. By using the Lyapunov stability theory, we show that under the proposed algorithm, the agents decision variables reach consensus and converge asymptotically to the optimal solution when the local objective functions are strongly convex with locally Lipschitz gradients.

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MS68

Differentially Private Distributed Resource Allocation via Deviation Tracking

This paper studies distributed resource allocation problem where all the agents cooperatively minimize the sum of their cost functions. To prevent private information from being disclosed, agents need to keep their cost functions private against potential adversaries and other agents. We first propose a completely distributed algorithm via deviation tracking that deals with constrained resource allocation problem and preserve differential privacy for cost functions by masking states and directions with decaying Laplace noise. Adopting constant stepsize, we prove that the proposed algorithm converges linearly in mean square. The linear convergence is established under the standard assumptions of Lipschitz gradients and strong convexity instead of the assumption of bounded gradients that is usually imposed in most existing works. Moreover, we show that the algorithm preserves differential privacy for every agents cost function and establish the trade-off between the privacy and the convergence accuracy. Furthermore, we apply the proposed algorithm to economic dispatch problem in IEEE-14 bus system to verify the theoretical results.

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MS69

Adaptive Step-Size Rule for Conditional Gradient Methods Minimizing Weakly Smooth Objective Functions

For conditional gradient methods solving a nonlinear optimization problem, the step-size rule is an important factor affecting the rate of convergence of the method. We focus on a composite-type optimization problem whose objective function is the sum of a weakly smooth function and a convex function with uniformly convex structure. We propose an adaptive backtracking to determine the step-size which does not require the parameters on the problem structure. It is shown that the proposed method has the same guarantee of the convergence rate as the exact line-search.

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MS69

Convergence Analysis under Consistent Error Bounds

In this talk, we introduce the notion of consistent error bound functions which provides a unifying framework for error bounds for multiple convex sets. This framework goes beyond the classical Lipschitzian and Holderian error bounds and includes, for example, the error bounds obtainable under the theory of amenable cones. One of the main results we prove is that the convergence rate of several algorithms for feasibility problems can be expressed explicitly in terms of the underlying consistent error bound function. This allows us to show new and old results related to the convergence rate of several projection algorithms and, also, of a damped Douglas-Rachford algorithm. Finally, applications to conic feasibility problems are also given and we show that a number of algorithms have convergence rates depending explicitly on the singularity degree of the problem.

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MS69

Bregman Proximal Algorithms for Composite and Finite-Sum Nonconvex Minimization Problems

The employment of Bregman divergences in splitting algorithms has been growing in popularity in the last few years. Firstly, the extra degree of freedom in the metric selection can lead to new algorithms or may provide new insights on known ones. Secondly, while many classical such schemes are bound to Lipschitz differentiability requirements (especially in the nonconvex setting), the recently introduced notion of “relative smoothness’ has considerably widened the range of problems that can be addressed. This talk deals with Bregman proximal algorithms in the fully nonconvex setting. The employment of the Bregman Moreau envelope as Lyapunov function leads to extremely simple and intuitive converge analyses that naturally extend to block-coordinate variants. Furthermore, continuity of the envelope allows one to design linesearch-type extensions that preserve oracle complexity and convergence properties of first-order (Bregman) splitting schemes, and yet can attain up to superlinear asymptotic rates when directions of quasi-Newton type are selected.

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MS70

Finite-Sample Guarantees for Wasserstein Distributionally Robust Optimization: Breaking the Curse of Dimensionality

Despite its recent empirical success, existing performance guarantees on Wasserstein distributionally robust optimization (DRO) are either overly conservative or plausible only in large sample asymptotics. In this paper, we develop a non-asymptotic analysis for Wasserstein DRO that gives the first finite-sample guarantee without suffering from the curse of dimensionality. Our results highlight the bias-variation trade-off intrinsic in Wasserstein DRO, which balances between the empirical risk and the variation of the loss, measured by the Lipschitz norm or gradient norm of the loss.

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MS70

A General Framework for Optimal Data-Driven Optimization

We propose a statistically optimal approach to construct data-driven decisions for stochastic programs. A data-driven decision is a function that maps training data to feasible actions. It can always be expressed as the minimizer of a surrogate optimization model constructed from the data, and its quality is measured by its out-of-sample risk. Another quality measure is its out-of-sample disappointment, which we define as the probability that the out-of-sample risk exceeds the optimal value of the surrogate optimization model. As the data-generating probability measure is unknown, we seek data-driven decisions that minimize the out-of-sample risk—simultaneously with respect to every conceivable probability measure—subject to an upper bound on the out-of-sample disappointment. We prove that such Pareto-dominant data-driven decisions exist if the unknown true probability measure belongs to a parametric ambiguity set whose parameters admit a sufficient statistic that satisfies a large deviation principle. We also prove that the surrogate optimization model generating the optimal data-driven decision is a distributionally robust program constructed from the sufficient statistic and the rate function of its large deviation principle. This result holds even if the original stochastic program is non-convex or the training data is non-i.i.d. It also reveals how the data-generating stochastic process impacts the ambiguity set of the optimal distributionally robust program.

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MS70

Taming the Sample Complexity in Minimizing Tail-risks via Importance-weighted Adversarial Sampling

Formulating objectives or constraints in terms of tail risk measures such as VaR/CVaR is known to incur a steep-price in terms of sample complexity, primarily due to (i) the rarity with which relevant risky samples are available, and (ii) the resulting amplification of estimation errors while performing optimization. Motivated by the evolving role of CVaR-based optimization models in proactively managing risks and in ensuring uniformly good (fair) performance across minority subpopulations, we consider accelerating them with an importance-weighted objective constructed from adversarial scenarios with high tail risks. The challenge of selecting this alternative sampling distribution is automated by means of a transformation that implicitly learns and replicates the concentration properties observed in less rare samples. This novel approach is guided by a large deviations principle that brings out the phenomenon of self-similarity of optimal importance sampling distributions. To the best of our knowledge, the proposed estimator is the first to attain asymptotically optimal variance reduction for a wide variety of optimization objectives, including those modeled with algorithmic feature-mapping tools such as kernels, neural networks, etc. We demonstrate applicability by considering portfolio optimization and contextual routing problems.

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MS70

A Nonparametric Algorithm for Optimal Stopping based on Robust Optimization

Optimal stopping is a class of stochastic dynamic optimization problems with applications in finance and operations management. In this paper, we introduce a new method for solving optimal stopping problems with known probability distributions. First, we use simulation to construct a robust optimization problem that approximates the stochastic optimal stopping problem to any arbitrary accuracy. Second, we characterize the structure of optimal policies for the robust optimization problem, which turn out to be simple and finite-dimensional. Harnessing this characterization, we develop exact and approximation algorithms for solving the robust optimization problem, which in turn yield policies for the stochastic optimal stopping problem. Numerical experiments show that this combination of robust optimization and simulation can find policies that match, and in some cases significantly outperform, those from state-of-the-art algorithms on low-dimensional, non-Markovian optimal stopping problems that arise from options pricing.

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MS71

MADAM: A Parallel Exact Solver for Max-Cut based on Semidefinite Programming and Admm

We present `MADAM`, a parallel semidefinite based exact solver for Max-Cut, a problem of finding the cut with maximum weight in a given graph. The algorithm uses branch and bound paradigm that applies alternating direction method of multipliers as the bounding routine to solve the basic semidefinite relaxation strengthened by a subset of hypermetric inequalities. The benefit of the new approach is less computationally expensive update rule for the dual variable with respect to the inequality constraints. We provide theoretical convergence of the algorithm, as well as extensive computational experiments with this method, to show that our algorithm outperformes current state-of-the-art approaches. Furthermore, by combining algorithmic ingredients from the serial algorithm we develop an efficient distributed parallel solver based on MPI.

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MS71

Singularity Degree and Error Bounds in Semidefinite Programming

Optimization algorithms for semidefinite programs (SDPs) terminate at a 'solution' where the residual of the optimality conditions is sufficiently small. However, such proposed solutions do not correspond to 'good solutions' in general. The Euclidean distance from the proposed 'solution' to the optimal set can be several orders of magnitude greater than the residual of the optimality conditions. Since the distance to the optimal set is generally unknown, such a discrepancy is very undesirable. In 2001, Jos Sturm introduced singularity degree as a way to explain this pathology. In particular, he showed that large singularity degree is a necessary property of SDPs that exhibit the pathology. In this presentation we show that, in some sense, large singularity degree is also a sufficient property for poor convergence of certain path following algorithms for SDP.

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MS71

An SDP-Based Approach for Minimum Sum-of-Squares Clustering

The minimum sum-of-squares clustering problem (MSSC) consists in partitioning n observations into k clusters in order to minimize the sum of squared distances from the points to the centroid of their cluster. Peng and Xia (2005) showed the equivalence of MSSC to 0-1 semidefinite programming (SDP). We propose a branch and bound algorithm for the underlying non-convex 0-1 SDP model to obtain exact solutions for real clustering data sets. In our algorithm, the lower bound is computed by using a cutting plane procedure where valid inequalities are iteratively added to the SDP relaxation. The upper bound is computed with the constrained version of k-means where the initial centroids are extracted by looking at the solution of the SDP relaxation. In both cases, in the branch and bound, we incorporate instance-level must-link and cannot-link constraints to express knowledge about which instances should or should not be grouped together. We manage to reduce the size of the problem at each level preserving the structure of the SDP problem itself. The obtained results show that the approach allows to successfully solve instances of medium and large sizes.

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MS72

Safely Learning Dynamical Systems by Conic Optimization

A fundamental challenge in learning to control an unknown dynamical system is to reduce model uncertainty by making measurements while maintaining safety. In this work, we formulate a mathematical definition of what it means to safely learn a dynamical system by sequentially deciding where to initialize the next trajectory. In our framework, the state of the system is required to stay within a given safety region under the (possibly repeated) action of all dynamical systems that are consistent with the information gathered so far. For our first two results, we consider the setting of safely learning linear dynamics. We present a linear programming-based algorithm that either safely recovers the true dynamics from trajectories of length one, or certifies that safe learning is impossible. We also give an efficient semidefinite representation of the set of initial conditions whose resulting trajectories of length two are guaranteed to stay in the safety region. For our final result, we study the problem of safely learning a nonlinear dynamical system. We give a second-order cone programming based representation of the set of initial conditions that are guaranteed to remain in the safety region after one application of the system dynamics.

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MS72

Convergence Rates of RLT and Lasserre-Type Hierarchies for the Generalized Moment Moment Problem over the Simplex

We consider the generalized moment problem over the simplex. This is a rich setting and it contains NP hard problems as special cases. Using the Reformulation-Linearization Technique (RLT) and Lasserre-type hierarchies, relaxations of this problem are introduced and analyzed. For both hierarchies the rate of convergence of $\mathcal{O}(1/r)$ is proved for the case in which the duality gap is zero and under the assumption of the existence of a dual optimal solution using a quantitative version of Polya's Positivstellensatz. Moreover, we show the introduced linear relaxation is a generalization of a hierarchy for minimizing forms of degree d over the simplex introduced by de Klerk, Laurent and Parrilo.

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MS72

The Copositive Way to Obtain Certificates of Non-Negativity

We show how to use certificates of non-negativity over the non-negative orthant (resp. a simplex) to obtain certificates of non-negativity over generic (resp. compact) semi-algebraic sets. To illustrate our method, we construct new structured (e.g., sparse) certificates of non-negativity over unstructured compact sets. Also, we derive a general positivstellensatz which allows us to prove the existence of certificates of non-negativity for any semialgebraic compact set, based on any class of non-negative polynomials such as SOS, DSOS, SDSOS, hyperbolic, SONC, and SAGE polynomials. Unlike typical proofs that make use of algebraic geometry tools, our proofs use convex analysis tools only.

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MS72

Lagrangean Duanlity in Polynomial Optimization

The Lagrangean function associated with an optimization problem has and continuous to be of the utmost importance to develop algorithmic solution approaches for optimization problems. This is particularly the case when the problem of interest is convex, as in that case, optimizing the Lagrangean function provides a dual problem (Lagrangean dual) to the primal (original) one, satisfying strong duality. Here, using techniques borrowed from both polynomial optimization, copositive programming, and algebraic geometry, we show that the classical Lagrangean function associated with a polynomial optimization problem can be used to obtain a Lagrangean dual of the problem that satisfies strong duality, even when the problem is non-convex, as long as some qualification assumptions on the problem's objective and constraints are satisfied.

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MS73

A Dynamic Alternating Direction of Multipliers for Nonconvex Minimization with Nonlinear Functional Equality Constraints

We consider the minimization of a broad class of nonsmooth nonconvex objective functions subject to nonlinear functional equality constraints where the data are only locally Lipschitz continuous. We introduce a specific proximal linearized alternating direction method of multipliers in which the proximal parameter is generated dynamically via an explicit and tractable backtracking procedure. We prove global convergence of the method when the problem's data is semialgebraic. Furthermore, as a byproduct of our approach, we also obtain novel global convergence guarantees for the iconic proximal gradient scheme.

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MS73

Convergent Nested Alternating Minimization Algorithms for Non-Convex Optimization Problems

We introduce a new algorithmic framework for solving non-convex optimization problems, which is called Nested Alternating Minimization, that aims at combining the classical Alternating Minimization technique with inner iterations of any optimization method. We provide global convergence analysis of the new algorithmic framework to critical points of the problem at hand, which to the best of our knowledge, is the first of this kind for nested methods in the non-convex setting. Central to our global convergence analysis is a new extension of classical proof techniques in the non-convex setting that allows for errors in the conditions. The power of our framework is illustrated with some numerical experiments that show the superiority of this algorithmic framework over existing methods.

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MS73

Faster Lagrangian-Based Methods in Convex Optimization

We aim at unifying, simplifying, and improving the convergence rate analysis of Lagrangian-based methods for convex optimization problems. We first introduce the notion of a nice primal algorithmic map, which plays a central role in the unification and the simplification of the analysis of all Lagrangian-based methods. Equipped with a nice primal algorithmic map, we then introduce a versatile generic scheme, which allows for the design and analysis of Faster LAGrangian (FLAG) methods with a new provably sublinear rate of convergence expressed in terms of functions values and feasibility violation of the original (non-ergodic) generated sequence. To demonstrate the power and versatility of our approach and results, we show that all well-known iconic Lagrangian-based schemes admit a nice primal algorithmic map, and hence share the new faster rate of convergence results within their corresponding FLAG.

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MS74

Max Affine Spline Models in Deep Learning Networks

We build a rigorous bridge between deep networks (DNs) and approximation theory via spline functions and operators. Our key result is that a large class of DNs can be written as a composition of max-affine spline operators (MASOs), which provide a powerful portal through which to view and analyze their inner workings. For instance, conditioned on the input signal, the output of a MASO DN can be written as a simple affine transformation of the input. This implies that a DN constructs a set of signal-dependent, class-specific templates against which the signal is compared via a simple inner product; we explore the links to the classical theory of optimal classification via matched filters and the effects of data memorization. Going further, we propose a simple penalty term that can be added to the cost function of any DN learning algorithm to force the templates to be orthogonal with each other; this leads to significantly improved classification performance and reduced overfitting with no change to the DN architecture. The spline partition of the input signal space that is implicitly induced by a MASO directly links DNs to the theory of vector quantization (VQ) and K-means clustering, which opens up new geometric avenue to study how DNs organize signals in a hierarchical fashion. To validate the utility of the VQ interpretation, we develop and validate a new distance metric for signals and images that quantifies the difference between their VQ encodings.

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MS74

Composite Difference-Max Programs for Modern Statistical Estimation Problems

Many modern statistical estimation problems are defined by three major components: a statistical model that postulates the dependence of an output variable on the input features; a loss function measuring the error between the observed output and the model predicted output; and a regularizer that controls the overfitting and/or variable selection in the model. We study the sampled version of this generic statistical estimation problem where the model parameters are estimated by empirical risk minimization, which involves the minimization of the empirical average of the loss function at the data points weighted by the model regularizer. In our setup we allow all three component functions to be of the difference-of-convex type and illustrate them with a host of commonly used examples, including those in continuous piecewise affine regression and in deep learning with piecewise affine activation functions. We describe a non-monotone majorization-minimization (MM) algorithm for solving the unified nonconvex, nondifferentiable optimization problem which is formulated as a specially structured composite dc program of the pointwise max type. Numerical results are presented to demonstrate the effectiveness of the proposed algorithm and the superiority of continuous piecewise affine regression over the standard linear model.

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MS74

Max-Affine Regression: Modeling and Leveraging Structure in High-Dimensional Convex Regression and its Relatives

The problem of fitting convex functions to data is ubiquitous, and has seen applications across the fields of operations research, finance, and control engineering. However, like most non-parametric problems, convex regression suffers from the curse of dimensionality: the number of samples required to achieve a prescribed error tolerance grows exponentially in the ambient dimension. In order to avoid the curse of dimensionality, we study the problem of "max-affine" regression, in which the underlying convex function is equipped with additional structure and can be written as the point-wise maximum of a small number of affine functions. This stylized model is already quite expressive, and includes, as a special case, the well-studied phase retrieval problem. Performing estimation under this class of models involves solving a non-convex, non-smooth optimization problem. We analyze an alternating minimization heuristic for this task, showing that it provably converges to the true model under some (flexible) random design assumptions. The algorithm needs to be appropriately initialized in order to ensure convergence, and we discuss some strategies for accomplishing this. We also discuss consequences for phase retrieval, and the related problems of convex set estimation from support function measurements. Joint work with Avishek Ghosh, Adityanand Guntuboyina, and Kannan Ramchandran.

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MS74

Fitting Tractable Convex Sets to Support Function Evaluations

The geometric problem of estimating an unknown compact convex set from evaluations of its support function arises in a range of scientific and engineering applications. Traditional approaches typically rely on estimators that minimize the error over all possible compact convex sets; in particular, these methods do not allow for the incorporation of prior structural information about the underlying set and the resulting estimates become increasingly more complicated to describe as the number of measurements available grows. We address these shortcomings by describing a framework for estimating tractably specified convex sets from support function evaluations. Our approach is based on estimators that minimize the error over structured families of convex sets that are specified as linear images of concisely described sets – such as the simplex or the spectraplex – in a higher-dimensional space that is not much larger than the ambient space. Convex sets parametrized in this manner are significant from a computational perspective as one can optimize linear functionals over such sets efficiently; they serve a different purpose in the inferential context of the present paper, namely, that of incorporating regularization in the reconstruction while still offering considerable expressive power.

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MS75

Robust Two-Stage Polynomial Optimization in Application to AC Optimal Power Flow

In this work we consider two-stage polynomial optimization problems under uncertainty. In the first stage, one needs to decide upon the values of a subset of optimization variables (control variables). In the second stage, the uncertainty is revealed and the rest of optimization variables (state variables) are set up as a solution to a known set of possibly non-linear equalities. This type of problems occurs, for instance, in optimization for dynamical systems, such as power systems. We combine several methods from the literature to verify robust feasibility of a given control solution under a semialgebraic uncertainty set. Moreover, we propose an iterative algorithm to build a sequence of (approximately) robustly feasible solutions with an improving objective value. At each iteration, the algorithm optimizes over a subset of the feasible set and uses linear approximations of the second-stage equalities while preserving the non-linearity of other constraints. The algorithm allows for additional simplifications in case of (possibly non-convex) quadratic problems under ellipsoidal uncertainty. We implement our approach for AC Optimal Power Flow (ACOPF) and demonstrate tests on Matpower instances.

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MS75

Compositions of Conically Averaged Operators

Many iterative optimization algorithms involve compositions of special cases of Lipschitz continuous operators, namely firmly nonexpansive, averaged and nonexpansive operators. The structure and properties of the compositions are of particular importance in the proofs of convergence of such algorithms. In this paper, we systematically study the compositions of further special cases of Lipschitz continuous operators. Applications of our results include compositions of scaled conically nonexpansive mappings, as well as the Douglas-Rachford and forward-backward operators when applied to solve certain structured monotone inclusion and optimization problems. Several examples illustrate and tighten our conclusions.

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MS75

Circumcenter Methods under the Bregman Distance

In this work, we generalize some classical identities on the distance and projections from the Euclidean distance to the general Bregman distance in Euclidean spaces. Under some conditions, we also propose particular backward and forward Bregman circumcenters of finite sets and specify the unique backward and forward Bregman psudo-circumcenters of finite sets. At last, we show the convergence of forward Bregman circumcenter methods under some conditions.

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MS75

Calculus Rules of the Generalized Kurdyka-Lojasiewicz Property

In this work, we propose several calculus rules of desingularizing functions of the generalized Kurdyka-Lojasiewicz (KL) property, which generalize Li and Pong's calculus rules of the KL exponent. In contrast, our results are more flexible since we do not assume desingularizing functions to have any specific form or differentiable. Taking advantage from this flexibility, one can find the exact modulus of the generalized KL property, which is the optimal desingularizing function and has various forms, or at least a small desingularizing function effectively. Examples are also given to show that our results are applicable to a broader class of functions than the known ones.

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MS76

Computationally-Efficient Robust Estimation in General f-divergences

In realizing the promise of massive datasets for statistical inference a primary concern is that of data quality. Large datasets are no longer carefully curated, are often collected in a decentralized, distributed fashion and are plagued with the complexities of heterogeneity, adversarial manipulations and outliers. Dealing with these issues are broadly the focus of robust statistics. This area has received much recent attention owing to the development of efficient algorithms for various basic robust estimation tasks under (potentially) adversarial contaminations. We show that these basic algorithmic ideas are much more generally applicable to settings where we have model-misspecification in a broad class of f-divergences. We illustrate the main ideas in three canonical problems, of mean estimation, covariance estimation and robust risk minimization.

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MS76

Large-Scale Methods for Distributionally Robust Optimization

We propose and analyze algorithms for distributionally robust optimization of convex losses with conditional value at risk (CVaR) and χ^2 divergence uncertainty sets. We prove that our algorithms require a number of gradient evaluations independent of training set size and number of parameters, making them suitable for large-scale applications. For χ^2 uncertainty sets these are the first such guarantees in the literature, and for CVaR our guarantees scale linearly in the uncertainty level rather than quadratically as in previous work. We also provide lower bounds proving the worst-case optimality of our algorithms for CVaR and a penalized version of the χ^2 problem. Our primary technical contributions are novel bounds on the bias of batch robust risk estimation and the variance of a multilevel Monte Carlo gradient estimator due to Blanchet and Glynn. Experiments on MNIST and ImageNet confirm the theoretical scaling of our algorithms, which are 9–36 times more efficient than full-batch methods.

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On the Effectiveness of Nonconvex Optimization in Reinforcement Learning

Recent years have witnessed a flurry of activity in solving reinforcement learning problems via nonconvex optimization. While conventional wisdom often takes a dim view of nonconvex optimization algorithms due to their susceptibility to spurious local minima, simple first-order optimization methods have been remarkably successful in practice. The theoretical footings, however, had been largely lacking until recently. In this talk, we make progress towards understandingthe efficacy of policy gradient type algorithms with softmax parameterization — a family of nonconvex optimization algorithms widely used in modern reinforcement learning.On the one hand, we demonstrate that softmax policy gradient methods can take exponential time to converge, even in the presence of a benign initialization and an initial state distribution amenable to optimization. On the other hand, we show that employing natural policy gradients and enforcing entropy regularization allow for fast global convergence.

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MS76

From Low Probability to High Confidence in Stochastic Convex Optimization

Standard results in stochastic convex optimization bound the number of samples that an algorithm needs to generate a point with small function value in expectation. More nuanced high probability guarantees are rare, and typically either rely on light-tail noise assumptions or exhibit worse sample complexity. In this work, we show that a wide class of stochastic optimization algorithms for strongly convex problems can be augmented with high confidence bounds at an overhead cost that is only logarithmic in the confidence level and polylogarithmic in the condition number. The procedure we propose, called proxBoost, is elementary and builds on two well-known ingredients: robust distance estimation and the proximal point method. We discuss consequences for both streaming (online) algorithms and offline algorithms based on empirical risk minimization.

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Computing Wasserstein Barycenters: Easy or Hard?

Averaging data distributions is a core subroutine throughout data science. Wasserstein barycenters (a.k.a. Optimal Transport barycenters) provide a natural approach for this problem that captures the geometry of the data, and are central to diverse applications in machine learning, statistics, and computer graphics. Despite considerable attention, it remained unknown whether Wasserstein barycenters can be computed in polynomial time. Our recent work provides a complete answer to this question and reveals a surprising curse of dimensionality. Joint work with Enric Boix-Adsera

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MS77

Optimal Transport Problems over Low and High Dimensional Euclidean Space

Optimal transport problems are often over structured metrics, such as the Euclidean space, where the cost is defined implicitly. In such a case, a near-linear time algorithm should be expected to run in time proportional to the description of the input is simply n, the number of points per set/support of the measures. This is in contrast to n^2, which is the input size when given an entire explicit cost matrix. In this talk, I will survey near-linear time algorithms for optimal transport problems in (mostly) Euclidean spaces, both in low and high dimensions.

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MS77

Differentiating through Optimal Transport

Computing or approximating an optimal transport cost is rarely the sole goal when using OT in applications. In most cases this relies instead on approximating that plan (or its application to another vector) to obtain its differentiable properties w.r.t. to its input. I will present in this talk recent applications that highlight this necessity, as well as possible algorithmic and programmatic solutions to handle such issues.

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MS77

Theory of Nearly Linear Time Algorithms for Optimal Transport

In this talk I will discuss recent advances in the theoretical complexity of computing the optimal transportation distance between two distributions. Over the past few years there have been several results on solving this problem in nearly linear time in different computational models. This talk will survey these recent advances and discuss recent work which shows that the problem can be solved to high precision in nearly linear time in certain settings.

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MS78

Infeasibility Detection with Primal-Dual Hybrid Gradient for Large-Scale Linear Programming

In this talk, we consider the problem of detecting infeasibility of large-scale linear programming problems using the primal-dual hybrid gradient method (PDHG) of Chambolle and Pock (2011). The literature on PDHG has mostly focused on settings where the problem at hand is assumed to be feasible. When the problem is not feasible, the iterates of the algorithm do not converge. In this scenario, we show that the iterates diverge at a controlled rate towards a well-defined ray. The direction of this ray is known as the infimal displacement vector v. The first contribution of our work is to prove that this vector recovers certificates of primal and dual infeasibility whenever they exist. Based on this fact, we propose a simple way to extract approximate infeasibility certificates from sequences generated by the iterates of PDHG. Our second contribution is to establish tight convergence rates for these sequences. We prove a convergence rate of $O\left(\frac{1}{k}\right)$, improving over the known rate of $O\left(\frac{1}{\sqrt{k}}\right)$. This rate is general and applies to any fixed-point iteration of a nonexpansive operator. Thus, it is a result of independent interest since it covers a broad family of algorithms, including, for example, ADMM. Further, we show that, under nondegeneracy assumptions, one of these sequences exhibits eventual linear convergence. Numerical experiments support our theoretical findings.

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MS78

iCrash: A Quadratic Penalty Algorithm for Linear Programming

Advanced basis start can be hugely beneficial for linear programming problems. This talk explores a crash starting technique for LP. The algorithm presented provides a way of computing a primal point that is often feasible and, in some cases, an approximate optimal solution. Crossover from this point is used to find a basic solution to start the simplex method or confirm optimality. iCrash is an iterative quadratic penalty algorithm with approximate subproblem minimization for large-scale sparse LP problems.

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MS78

Practical Large-Scale Linear Programming using Primal-Dual Hybrid Gradient

We present PDLP, a practical first-order method for linear programming (LP) that can solve to the high levels of accuracy that are expected in traditional LP applications. In addition, it can scale to very large problems because its core operation is matrix-vector multiplications. PDLP is derived by applying the primal-dual hybrid gradient (PDHG) method, popularized by Chambolle and Pock (2011), to a saddle-point formulation of LP. PDLP enhances PDHG for LP by combining several new techniques with older tricks from the literature; the enhancements include diagonal preconditioning, presolving, adaptive step sizes, and adaptive restarting. PDLP compares favorably with SCS on medium-sized instances when solving both to moderate and high accuracy. Furthermore, we highlight standard benchmark instances and a large-scale application (PageRank) where our open-source prototype of PDLP outperforms a commercial LP solver. The prototype of PDLP is written in Julia and available at https://github.com/google-research/FirstOrderLp.jl.

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MS78

Eclipse: An Extreme-Scale Linear Program Solver for Web-Applications

Key problems arising in web applications (with millions of users and thousands of items) can be formulated as linear programs involving billions to trillions of decision variables and constraints. Despite the appeal of linear program (LP) formulations, solving problems at these scales appear to be well beyond the capabilities of existing LP solvers. Often ad-hoc decomposition rules are used to approximately solve these LPs, which have limited optimality guarantees and may lead to sub-optimal performance in practice. In this work, we propose a distributed solver that solves a perturbation of the LP problems at scale via a gradient-based algorithm on the smooth dual of the perturbed LP. The main workhorses of our algorithm are distributed matrix-vector multiplications and efficient projection operations on distributed machines. Experiments on real-world data show that our proposed LP solver, ECLIPSE, can solve problems with 10^{12} decision variables.

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MS79

Regularization in Decomposition Methods for Global Optimization of Mixed-Integer Nonlinear Programming

The Outer-approximation (OA) method is one of the most successful decomposition methods for MINLP, where an optimal solution is found by solving MILP and NLP subproblems. Recently, Kronvist, Bernal, and Grossmann proposed using regularization ideas for MINLP[Kronqvist, J., Bernal, D. E., & Grossmann, I. E. (2020). Using regularization and second order information in outer approximation for convex MINLP. Mathematical Programming, 180(1), 285-310.]. Inspired by the regularization method for continuous convex problems, the authors proposed a method that, by solving an additional regularization MIQP in each iteration, leads to a reduction in the total OA iterations and total algorithmic runtime. In this work, we propose using MILP regularization subproblems to achieve the iteration number reduction and avoid the solution of expensive MIQP subproblems. Both the global version of OA and the regularization approaches, with MIQP and MILP subproblems, have been implemented as part of the open-source Python toolkit MindtPy. This toolkit automatically performs the decomposition and solves the subproblems via Pyomo. MindtPy provides the end-user a seamless way of combining decomposition algorithms, allowing for an easy way of addressing challenging MINLP instances. Here we present the details of this implementation, together with the theoretical and algorithmic advances required by the methods above, and a benchmark of our tool comparing it with other solution methods for MINLP.

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MS79

Tight Piecewise Relaxations for Global Optimiza-

tion of MINLPs

MINLPs arise in practical applications such as synthesis of process and water networks, energy infrastructure networks, to name a few. Efficient algorithms to solve such optimization problems to global optimality is a key to addressing these applications. We present a MILP-based formulation of a piecewise, polyhedral relaxation of multilinear terms based on term-wise convex hull representations. We also present a few valid inequalities which tighten these relaxations for the summation of multilinear terms with shared products of variables. Recovering feasible solutions for MINLPs with multilinear terms using a MILP-based approach is also presented based on an sos-2-type formulation. Finally, we present an adaptive partitioning-based algorithm implemented in "Alpine", a JuMP-based global optimization solver which leverages MILP-based approaches, constraint programming techniques and aforementioned efficient formulations. Computational results will compare the performance of Alpine on various MINLPLib instances in comparison to other state-of-the-art global solvers.

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MS79

Minimum Linearization of Multilinear Programs

Linear Programming (LP) relaxations are widely employed in the global optimization of Multilinear Programs (MLPs). The LP relaxation is derived by introducing additional variables that represent bilinear products and including concave and convex envelopes. The size of the LP relaxation depends on the heuristic employed to identify the collection of variables to add. In this paper, we introduce the first approach for identifying the smallest size LP for a given MLP, by investigating a Mixed Integer Program (MIP) model that solves a specialized decision diagram representation where linearizations are encoded as in-trees. Our results on a collection of benchmarks indicate that the MIP can find smaller linearizations (up to 20% reduction in number of variables) than the standard approach, and the quality of the relaxation bounds varies greatly among different minimum size linearizations.

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MS79

Nonconvex Quadratic Cuts for Global Optimization of Mixed Integer Quadratic Programs

Nonconvex quadratic programs (QPs) and mixed-integer quadratic programs (MIQPs) arise in a wide variety of scientific and engineering applications including facility location, quadratic assignment, molecular conformation and max-cut problems. In this talk, we introduce a new family of quadratically constrained programming (QCP) relaxations which are derived via nonconvex quadratic cuts. However, the nonconvex cuts in conjuncrtion with equality constraints yield convex QCP relaxations for the MIQP. In order to construct these quadratic cuts, we solve a separation problem involving a linear matrix inequality with a special structure that allows the use of specialized solution algorithms. We investigate the theoretical properties of the proposed relaxations and show that they are an outer-approximation of a semi-infinite convex program which under certain conditions is equivalent to a particular semidefinite program. We implement the new quadratic relaxations in the global optimization solver in BARON. We test our implementation by conducting an extensive computational study on a large collection of problems. Numerical results show that the new quadratic relaxations lead to a significant improvement in the performance of BARON, resulting in a new version of this solver which outperforms other state-of-the-art solvers such as CPLEX and GUROBI for many of our test problems.

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MS80

Integer Programming for Causal Structure Learning in the Presence of Latent Variables

Causal graphs are graphical models representing dependencies and causal relationships between a set of variables. One class of the most common causal graphs, known as Bayesian networks (BNs), is modeled by directed acyclic graphs (DAGs) in which a direct causal relationship between two nodes is captured by a directed edge. In this work we extend a previous state-of-the-art Integer Programming (IP) based DAG structure learning method GOBNILP and provide an IP based method for learning causal structures in the presence of latent variables. In particular, we give an IP formulation for the problem of finding a maximum weight ancestral acyclic directed mixed graph (ADMG), and generalize the DAG-related inequalities used in GOBNILP for this purpose. Our method is the first exact score based method for learning ADMGs, and it performs competitively with existing structure based methods.

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MS80

Fair Binary Classification using Integer Program-

ming

We consider the problem of building Boolean rule sets in disjunctive normal form (DNF), an interpretable model for binary classification, subject to fairness constraints. We formulate the problem as an integer program that maximizes classification accuracy with explicit constraints on equality of opportunity. A column generation framework, with a novel formulation, is used to efficiently search over exponentially many possible rules, eliminating the need for heuristic rule mining. Compared to other interpretable machine learning algorithms, our method produces interpretable classifiers that have superior performance with respect to the fairness metric.

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MS80

Linear Programming Relaxations for Joint Object Matching

Object matching techniques are widely used in computer vision. While there is a rich literature on finding isomorphisms between pair of objects, the problem of joint object matching, that is, finding consistent maps among all pairs of objects within a collection is not well understood. We study the problem of joint object matching in which the objects are partially similar and the input is possibly incomplete. The only existing convex relaxations for this problem are SDP relaxations which are quite expensive to solve. We formulate this problem as an integer program and propose a linear programming relaxation for it. Subsequently, we study theoretical properties of the proposed LP under some popular generative models. Finally computational experiments will be presented.

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MS80

Decision Forests and Multilinear Polytopes

In this paper, we study the simultaneous convexification of a multilinear set over the cartesian product of simplices: $\left\{(x_1,\cdots,x_n,y)\in\Delta_{K_1}\times\cdots\times\Delta_{K_n}\times\mathbb{R}^L \;\middle|\; y_\ell=\prod_{i=1}^n\left(\sum_{j\in J_{i,\ell}} x_{i,j}\right),\ \forall \ell\in\{1,\ldots,L\}\right\}$ where $\Delta_K := \{(z_1,\ldots,z_{K+1})\in\mathbb{R}_+^{K+1} : 1^\intercal z = 1\}$ and $J_{i,\ell}$ is a nonempty subset of $\{1,\ldots,K_i\}$. We obtain explicit descriptions of the multilinear polytope under certain conditions. While the descriptions require an exponential number of inequalities in the (x,y)-space, we show that the separation takes a polynomial time. The result can be applied to the optimization of a decision forest to achieve an improved formulation.

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MS81

SALR: Sharpness-Aware Learning Rates for Improved Generalization

In an effort to improve generalization in deep learning, we propose SALR: a sharpness-aware learning rate update technique designed to recover flat minimizers. Our method dynamically updates the learning rate of gradient-based optimizers based on the local sharpness of the loss function. This allows optimizers to automatically increase learning rates at sharp valleys to increase the chance of escaping them. We demonstrate the effectiveness of SALR when adopted by various algorithms over a broad range of networks. Our experiments indicate that SALR improves generalization, converges faster, and drives solutions to significantly flatter regions.

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MS81

Halting Time is Predictable for Large Models: A Universality Property and Average-Case Analysis

In this talk, I will present a framework for performing average-case analysis in the large dimensional regime. Average-case analysis computes the complexity of an algorithm averaged over all possible inputs. Compared to worst-case analysis, it is more representative of the typical behavior of an algorithm, but remains largely unexplored in continuous optimization. One difficulty is that the analysis can depend on the probability distribution of the inputs to the model. However, I will show that this is not the case for a class of large-scale problems trained with first-order methods including random least squares and one-hidden layer neural networks with random weights. In fact, the halting time exhibits a universality property: it is independent of the probability distribution. With this barrier for average-case analysis removed, I will present the first explicit average-case convergence rates showing a tighter complexity not captured by traditional worst-case analysis.

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MS81

Trust-region Newton-CG with Strong Second-order Complexity Guarantees for Nonconvex Optimization

Worst-case complexity guarantees for nonconvex optimization algorithms have been a topic of growing interest. Multiple frameworks that achieve the best known complexity bounds among a broad class of first- and second-order strategies have been proposed. These methods have often been designed primarily with complexity guarantees in mind and, as a result, represent a departure from the algorithms that have proved to be the most effective in practice. In this talk, we consider the popular trust-region Newton-Conjugate-Gradient (Newton-CG) method, one of the most popular paradigms for solving nonconvex optimization problems. We first study the behavior of the truncated conjugate gradient method when applied to a trust-region subproblem. We then incorporate this algorithm within a trust-region framework that hews closely to the classical Steihaug-Toint approach. The complexity properties of this method match the best known results in terms of iteration and computational complexity. A numerical comparison on a standard benchmark test set illustrates that our newly proposed method retains the attractive practical behavior of classical trust-region Newton-CG algorithms. Joint work with Frank E. Curtis, Daniel P. Robinson and Stephen J. Wright.

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MS81

Stochastic Variance-reduced Prox-linear Algorithms for Nonconvex Composite Optimization

We consider the minimization of composite functions of the form f(g(x)) + h(x), where f and h are convex and g is a smooth vector mapping. In addition, we assume that g is either the average of a large number of component mappings or the expectation over a family of random component mappings. We propose a class of stochastic prox-linear algorithms with variance reduction for solving such problems. We bound their sample complexities under four different settings, depending on f being nonsmooth or smooth and g being a finite sum or an expectation. In all four settings, we obtain improved (when f is nonsmooth) or matching (when f is smooth) sample complexities over the best known results.

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MS82

Layer VQE: Near Term Quantum Algorithm for Combinatorial Optimization

Combinatorial optimization on near-term quantum devices is a promising path to demonstrating quantum advantage. However, the capabilities of these devices are constrained by high noise levels and limited error-mitigation. In this paper, we propose an iterative Layer-VQE (L-VQE) approach, inspired by Variational Quantum Eigensolver (VQE). We present a large-scale numerical study, simulating circuits with up to 40 qubits and 352 parameters, that demonstrates the potential of the proposed approach. We evaluate quantum optimization heuristics on the problem of detecting multiple communities in networks, for which we introduce a novel qubit-frugal formulation. We numerically compare L-VQE to QAOA and demonstrate that QAOA achieves lower approximation ratios while requiring significantly deeper circuits. We show that L-VQE is more robust to sampling noise and has a higher chance of finding the solution as compared to standard approaches. Our simulation results show that L-VQE performs well under realistic hardware noise.

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MS82

Outperforming QAOA on MaxCut with Fast Classical Hyperplane Rounding Algorithms

In recent years, several classical algorithms have been presented which beat the p=1 Quantum Approximate Optimization Algorithm (QAOA) approximation guarantee for Max Cut on d-regular, triangle-free graphs. However, these algorithms require tricks and numerical analysis for certain values of the vertex degree, d. In this talk, we present a simple vector rounding algorithm for regular, high girth graphs which beats QAOA for all d. Every vertex in the graph is assigned a vector, which gives a valid solution to the standard Max Cut relaxation semidefinite program (SDP). Then the vectors are rounded using the Goemans-Williamson SDP rounding scheme to generate a cut. Our algorithm does not require solving an SDP and runs in linear time. The guaranteed expected value is larger than that of the classical state of the art as a function of the degree and girth of the graph. Finally, we will discuss other applications of our algorithm and consequences for QAOA.

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MS82

Warm-Starting Quantum Optimization

There is an increasing interest in quantum algorithms for problems of combinatorial optimization. Classical solvers for such problems employ relaxations, which replace binary variables with continuous ones, for instance in the form of higher-dimensional matrix-valued problems (semidefinite programming). Under the Unique Games Conjecture, these relaxations often provide the best approximation ratios available classically in polynomial time. Here, we discuss how to warm-start quantum optimization with an initial state corresponding to the solution of a relaxation of a combinatorial optimization problem and how to analyze properties of the associated quantum algorithms. We illustrate this in the context of portfolio optimization, where our results indicate that warm-starting the Quantum Approximate Optimization Algorithm (QAOA) is particularly beneficial at low depth. Likewise, Recursive QAOA for MAXCUT problems shows a systematic increase in the size of the obtained cut for fully connected graphs with random weights, when Goemans-Williamson randomized rounding is utilized in a warm start. It is straightforward to apply the same ideas to other randomized-rounding schemes and optimization problems.

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MS83

Multistage Stochastic Programming with Optimal Stopping

The theory of optimal stopping finds interesting applications in house selling, one-armed bandit, option trading, etc. In this talk, we present a general formulation of multistage stochastic programming that incorporates optimal stopping. This formulation can be solved, as usual, by writing down the Bellman equation and applying dynamic programming. Our focus will be on applications and computational aspects of the formulation.

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MS83

Bounds for Multistage Mixed-Integer Distributionally Robust Optimization

Multistage mixed-integer distributionally robust optimization (DRO) forms a class of extremely challenging problems since their size grows exponentially with the number of stages. One way to model the uncertainty in a multistage setting, is by creating sets of conditional distributions (the so called conditional ambiguity sets) on a finite scenario tree and requiring that such a distributions remain close to a nominal conditional distribution via phi-divergences (e.g. variation distance, Cressie-Read power divergence etc.) or Wasserstein distance. In this talk, new lower bounding criteria for such a class of difficult decision problems are provided through scenario grouping using the conditional ambiguity sets associated to some commonly used phi-divergences and Wasserstein distance. We also show that, for a special case of Cressie-Read Power divergence, another way to obtain the same results is to consider the risk envelope corresponding to the ambiguity set. Our approach does not require any special problem structure such as convexity and linearity, therefore it can be applied to a wide range of DRO problems including two-stage and multistage, with or without integer variables. Extensive numerical results on a mixed integer multi-stage risk-averse production problem are finally presented showing the efficiency of the proposed approach over different choices of partition strategies, phi-divergences and risk levels.

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MS83

Capacity Planning using JuDGE

We describe JuDGE, a Julia package for solving multistage stochastic capacity planning problems. JuDGE applies Dantzig-Wolfe decomposition to multi-horizon scenario trees, whereby the master problem solves a multistage stochastic program, and subproblems optimize operations that are (possibly) subject to random effects. We illustrate JuDGE by applying it to investment in renewable electricity generation and transmission capacity in New Zealand.

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MS83

Complexity for Multistage Distributionally Robust Dual Dynamic Programming

In this talk, we present a novel algorithmic study and complexity analysis of distributionally robust convex optimization (DR-MCO), which encompasses multistage stochastic convex optimization (MSCO) and multistage robust convex optimization (MRCO) as special cases. The proposed cutting-plane algorithmic framework unifies and generalizes the existing robust and stochastic dual dynamic programming algorithms. We discuss the technique of Lipschitz regularization that enables the algorithms to handle fast growth of Lipschitz constants of value functions, and problems without relatively complete recourse, under mild assumptions. Further, we consider a nonsequential version of the algorithm, in addition to the usual sequentially executed dual dynamic programming algorithms. Assuming single stage subproblem oracles, we then provide a thorough complexity analysis of the new algorithms with both upper complexity bounds and a matching lower bound, quantifying the dependence on the number of stages, the dimensions of state spaces and other regularity characteristics of the problem. Various numerical examples are included to illustrate the algorithms and complexity analysis, including DR-MCO with finitely supported distributions, DR-MCO with Wasserstein ambiguity sets, MSCO with empirical distributions and MRCO with polyhedral uncertainty sets.

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MS84

Optimization for Deep Learning: Challenges, Insights and Solutions

Modern deep learning problems pose new challenges that classical optimization approaches are not necessarily well suited to solve. In this talk I give an overview of the challenges involved at training large models in computer vision and natural language processing. I will describe potential solutions and interesting research avenues in this area.

I will also discuss how the structure and initialization of neural networks can be modified to improve conditioning.

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MS84

Homeomorphic-Invariance of EM: Non-Asymptotic Convergence in KL Divergence for Exponential Families via Mirror Descent

Expectation maximization (EM) is the default algorithm for fitting probabilistic models with missing or latent variables, yet we lack a full understanding of its non-asymptotic convergence properties. Previous works show results along the lines of "EM converges at least as fast as gradient descent" by assuming the conditions for the convergence of gradient descent apply to EM. This approach is not only loose, in that it does not capture that EM can make more progress than a gradient step, but the assumptions fail to hold for textbook examples of EM like Gaussian mixtures. In this work we first show that for the common setting of exponential family distributions, viewing EM as a mirror descent algorithm leads to convergence rates in Kullback-Leibler (KL) divergence. Then, we show how the KL divergence is related to first-order stationarity via Bregman divergences. In contrast to previous works, the analysis is invariant to the choice of parametrization and holds with minimal assumptions. We also show applications of these ideas to local linear (and superlinear) convergence rates, generalized EM, and non-exponential family distributions.

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MS84

Rethinking Stochastic Optimization for Over-parameterized Models

Modern machine learning focuses on training highly expressive over-parametrized models that are able to fit or interpolate the data completely, resulting in zero training loss. When training such models, we show that stochastic gradient descent (SGD) can achieve faster rates of convergence, matching those of full-batch deterministic gradient descent. We exploit this interpolation property to propose a stochastic line-search scheme to set the SGD step-size in each iteration; thus alleviating the need to manually tune it. Under the interpolation setting, we prove that SGD equipped with stochastic line-search achieves fast convergence without requiring knowledge of any problem-dependent constants. Experimentally, we show that SGD with line-search outperforms state-of-the-art optimization methods on standard benchmarks. Next, we consider incorporating second-order information when training over-parametrized models. Specifically, we show that the regularized sub-sampled Newton method (R-SSN) achieves global linear convergence with constant batch size. By growing the batch size for both the sub-sampled gradient and Hessian, we show that R-SSN can converge at a quadratic rate in a local neighborhood of the solution. We empirically demonstrate that stochastic second-order methods can result in faster convergence compared to common first-order methods.

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MS85

Performance Improvement Strategies in Direct Search for Multiobjective Optimization

Direct Search has been successfully used in multiobjective optimization, allowing to compute good quality approximations to the complete Pareto front of a given problem, for local and global derivative-free optimization. These algorithms have a well-supported convergence analysis and have proved to be competitive with other classes of multiobjective optimization solvers, not only in academic test sets, but also in real applications. The algorithmic structure of a direct search method is organized in a search step and a poll step, performed after the selection of an iteration center. Different strategies can be used for this center selection, and parallel approaches can allow the selection of more than one iteration center at a time. Minimizers of surrogate models, built by reusing points already evaluated, can also enhance the numerical performance of these methods. In this work, we detail the previous strategies and present numerical results that support their value, both in an academic test set and in a chemical engineering application.

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MS85

Gradient and Hessian Approximation Techniques in Derivative-Free Optimization

In this presentation, derivative-free approximation techniques to approximate the gradient and the Hessian are discussed. Error bounds for the underdetermined, determined and overdetermined cases are introduced. A novel Hessian approximation technique called the *nested-set Hessian* is provided. It is proven that the nested-set Hessian requires $(n+1)(n+2)/2$ function evaluations to accurately approximate the Hessian and it is demonstrated how to build a *minimal poised set for nested-set Hessian computation*.

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MS85

Applying Complex-Step Derivative Approximations in Model-Based Derivative-Free Optimization

Derivative-free optimization refers to the optimization of functions without the analytical knowledge of the functions expressions or derivatives. Model-based DFO methods solve this by constructing models of the objective functions. In this work, we numerically address the question, Can using complex numbers in constructing models provide better results in model-based derivative-free optimization? We provide several complex-variable based methods to approximate gradients and Hessians, then provide numerical error bounds for these methods . We use these methods within Newtons optimization algorithm. The results obtained from the complex-step derivative approximation methods are then compared to the optimization results obtained by real-step quadratic models. Algorithm performance is analysed on the basis of number of function evaluations called by a model, number of iterations or the step size required for satisfactory precision. Results suggest that a complex-step approach can improve model-based DFO algorithmic performance.

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MS86

Doubleton Projections in Real Hilbert Spaces

Suppose X is a real Hilbert space. We say a set $C \subseteq X$ admits a Continuous Doubleton Projection if there is a point $x \in X \setminus C$ that projects onto exactly two points of C, and that the metric projection map P_C is upper-semicontinuous at x. We present two conditions equivalent to C failing to admit a doubleton projection: a property related to (but stronger than) connectedness called B°-Connectedness, and a property we call Locally-Determined Set Curvature. These results tells us some non-trivial geometric facts about Chebyshev sets in real Hilbert Spaces. Such sets are the subject of a long-standing open problem known as the Chebyshev Conjecture.

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MS86

Convex Analysis of Minimal Time Functions and Signed Minimal Time Functions

In this talk we first consider the class of minimal time functions well known in the literature in the setting of locally convex topological vector spaces. Then we introduce and present general and generalized differential properties of a new class of functions called the signed minimal time function, which is a generalization of the signed distance function. (This talk is based on the joint work with D. V. Cuong, B. Mordukhovich, and M. Wells)

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MS86

Finding Best Approximation Pairs for Two Intersections of Closed Convex Sets

The problem of finding a best approximation pair of two sets, which in turn generalizes the well known convex feasibility problem, has a long history that dates back to work by Cheney and Goldstein in 1959. In 2018, Aharoni, Censor, and Jiang revisited this problem and proposed an algorithm that can be used when the two sets are finite intersections of halfspaces. Motivated by their work, we present alternative algorithms that utilize projection and proximity operators. Numerical experiments indicate that these methods are competitive and sometimes superior to the one proposed by Aharoni et al.

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MS86

Directional Necessary Optimality Conditions for Bilevel Programs

The bilevel program is an optimization problem where the constraint involves solutions to a parametric optimization problem. It is well-known that the value function reformulation provides an equivalent single-level optimization problem but it results in a nonsmooth optimization problem which never satisfies the usual constraint qualification such as the Mangasarian-Fromovitz constraint qualification (MFCQ). In this paper we show that even the first order sufficient condition for metric subregularity which is in general weaker than MFCQ fails at each feasible point of the bilevel program. We introduce the concept of directional calmness condition and show that under the directional calmness condition, the directional necessary optimality condition holds. While the directional optimality condition is in general sharper than the non-directional one, the directional calmness condition is in general weaker than the classical calmness condition and hence is more likely to hold. We perform the directional sensitivity analysis of the value function and propose the directional quasi-normality as a sufficient condition for the directional calmness. An example is given to show that the directional quasi-normality condition may hold for the bilevel program.

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MS87

Curriculum Learning for Interdiction Games

In this work, we focus on an integer programming game played between a defender and an attacker, the Multilevel Critical Node problem. Broadly studied in the literature, the Critical Node problem investigates graphs' reliability, robustness and impermeability against the removal of edges or vertices. Hence, the multilevel version of this problem adds a dynamic component where a defender not only anticipates a potential network attack but she can also react after it. Such settings are known as defender-attacker-defender games. Our game is known to be at least Σ_2^p-hard for directed graphs and Σ_3^p-hard for weighted graphs. This motivated us to develop a curriculum learning approach for the automatic design of greedy heuristics for multilevel budgeted combinatorial problems. Besides the description of our game and methodology, we will present computational results reflecting the effectiveness of our framework and the research venues it opens.

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MS87

An Overview and the Benefits of Different Optimization Techniques

Optimization is a fundamental tool in many areas of science and engineering; it can be applied in a wide range of problems covering different disciplines by utilizing machine learning techniques. There are a large number of proposed optimization techniques; this number is expected to increase due to the No-Free-Lunch (NFL) theorem. Therefore, this presentation briefly defines the optimization problem and describes the different types of optimization techniques such as evolutionary, physics-based, and swarm-based algorithms and clarifies some conflicting terms. It also lists different types of problems that can be efficiently solved using these techniques; and shows the advantages of using the optimization phases in different applications.

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MS88

Riemannian Proximal Gradient Methods

We consider solving nonconvex and nonsmooth optimization problems with Riemannian manifold constraints. Such problems have received considerable attention due to many important applications such as sparse PCA, sparse blind deconvolution, robust matrix completion. Many of the applications yield composite objectives. In the Euclidean setting, the proximal gradient method and its variants have been viewed as excellent methods for solving nonconvex nonsmooth problems with composite cost functions. However, in the Riemannian setting, the related work is still limited. In this talk, we briefly review existing nonsmooth optimization methods on Riemannian manifolds, in particular, the proximal gradient method on manifolds. We develop and analyze a Riemannian proximal gradient method. It is shown that the global convergence is obtained for the Riemannian proximal gradient method under mild assumptions. The O(1/k) convergence rates are established for the method and its variant under more assumptions. Local convergence rate analysis is further given using Kurdyka-Lojasiewicz property. A practical algorithm is also proposed. Two models in sparse PCA are used to demonstrate the performance of the proposed methods.

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MS88

Polar Decomposition Based Algorithms on the Product of Stiefel Manifolds with Applications in Tensor Approximation

In this paper, we propose a general algorithmic framework to solve a class of optimization problems on the product of complex Stiefel manifolds based on the matrix polar decomposition. We establish the weak convergence, global convergence and linear convergence rate of this general algorithmic approach using the Lojasiewicz gradient inequality and the Morse-Bott property. This general algorithm and its convergence results are applied to the simultaneous approximate tensor diagonalization and simultaneous approximate tensor compression, which include as special cases the low rank orthogonal approximation, best rank-1 approximation and low multilinear rank approximation for higher order complex tensors. It turns out that well-known algorithms such as LROAT and HOPM are both special cases of this general algorithmic framework, and our convergence results subsume the results found in the literature designed for those special cases.

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MS88

New Class of Riemannian Conjugate Gradient Methods

One of the main differences between Riemannian conjugate gradient (R-CG) methods, i.e., CG on Riemannian manifolds, and traditional Euclidean CG methods is the computation of search directions. While earlier studies used the parallel translation to compute search directions in R-CG, the concept of vector transport, which can be considered an approximation of the parallel translation, was proposed to obtain numerically more efficient R-CG. However, recent studies have shown that mappings other than vector transports, e.g., inverse retractions, can also be used in R-CG. In this talk, we discuss a new class of R-CG, in which we use general mappings containing vector transports and inverse retractions as special cases to compute search directions. We specify what conditions should be imposed on the proposed mappings and provide a convergence analysis for the proposed R-CG.

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MS88

Weakly Convex Optimization over Stiefel Manifold using Riemannian Subgradient-Type Methods

In this talk, we present a family of Riemannian subgradient-type methods to solve a class of non-smooth optimization problems over the Stiefel manifold, in which the objective function is weakly convex in the ambient Euclidean space. We show that these methods have an iteration complexity of $\mathcal{O}(\epsilon^{-4})$. Furthermore, we establish the local linear convergence of Riemannian subgradient and incremental subgradient methods when the problem at hand further satisfies a sharpness property and the algorithms are properly initialized and use geometrically diminishing stepsizes. To the best of our knowledge, these are the first convergence guarantees for using Riemannian subgradient-type methods to optimize a class of non-convex non-smooth functions over the Stiefel manifold.

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MS90

Reformulation-Perspectification-Technique for Robust Optimization with Convex Uncertainty

Robust convex constraints are difficult to handle since finding the worst-case scenario is equivalent to maximizing a convex function. In this talk, we propose a new approach to deal with such constraints that unifies approaches known in the literature and extends them in a significant way. The extension is either obtaining better solutions than the ones proposed in the literature, or obtaining solutions for classes of problems unaddressed by previous approaches. Our solution is based on RPT and can be applied to general convex inequalities and general convex uncertainty sets. It generates a sequence of conservative approximations which can be used to obtain both upper- and lower- bounds for the optimal objective value. We illustrate the numerical benefit of our approach on a robust control and robust geometric optimization example.

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MS90

Reformulation-Perspectification-Technique: General Methodology

We introduce a novel Reformulation-Perspectification Technique (RPT) to obtain convex approximations of nonconvex continuous optimization problems. RPT consists of two steps, those are, a reformulation step and a perspectification step. The reformulation step generates redundant nonconvex constraints from pairwise multiplication of the existing constraints. The perspectification step then convexifies the nonconvex components by using perspective functions. The proposed RPT extends the existing Reformulation-Linearization Technique (RLT) in two ways. First, it can multiply constraints that are not linear or not quadratic, and thereby obtain tighter approximations than RLT. Second, it can also handle more types of nonconvexity than RLT.

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MS90

Reformulation-Perspectification-Technique for Conic Constraints

We demonstrate the applicability of the Reformulation-Perspectification-Technique (RPT) by extensively analyzing all 15 possibilities of pairwise multiplication of the five basic cone constraints (linear cone, second-order cone, power cone, exponential cone, semi-definite cone). For several of these 15 possibilities there are many ways to perform the perspectification step, and we discuss how to obtain the best one. We also show that the conic reformulation of the problem obtained after applying RPT to the original optimization problem is the same as RPT applied to the conic reformulation of the original optimization problem. Finally, we show that many well-known RLT based results can also be obtained and extended by applying RPT.

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MS91

On Solving Dynamical Nash Games using the Pontryagin Maximum Principle

The sequential quadratic Hamiltonian (SQH) method is a new efficient and robust variant of the successive approximations strategy for solving optimal control problems. In this talk, the development of this method for solving differential Nash games is discussed, with a focus on linear-quadratic problems. In addition, the case of a game with non-smooth objectives is also considered to demonstrate the larger applicability of the proposed computational framework.

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MS91

Nash Equilibria and Bargaining Solutions of Differential Games

Systems with a bilinear state-control structure arise in many applications in, e.g., biology, economics, physics, where competition between different species, agents, and forces needs to be modelled. For this purpose, the concept of Nash equilibria (NE) appears appropriate, and the building blocks of the resulting differential Nash games are different control functions associated with different players that pursue different non-cooperative objectives. In this framework, existence of Nash equilibria is proved and computed with a semi-smooth Newton scheme combined with a relaxation method. Further, a related Nash bargaining (NB) problem is discussed. This aims at determining an improvement of all players objectives with respect to the Nash equilibria. Results of numerical experiments successfully demonstrate the effectiveness of the proposed NE and NB computational framework.

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MS91

A Nash Games Framework to Control Pedestrian Behavior

In this talk, we present a new approach to modeling pedestrians avoidance dynamics based on a Fokker-Planck Nash game framework. In this framework, two interacting pedestrian are considered, whose motion variability is modeled through the corresponding probability density functions (PDFs) governed by Fokker-Planck equations. Based on these equations, a Nash differential game is formulated where the game strategies represent controls aiming at avoidance by minimizing appropriate collision cost functionals. Existence of Nash equilibria solutions is proved and characterized as solution to an optimal control problem that is solved numerically. Results of numerical experiments are presented that successfully compare the computed Nash equilibria to output of real experiments (conducted with humans).

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MS92

Geometric Convex-Hull Proofs: A Structured Approach and Integer Extensions

In the present work, we consider Zuckerberg's method for geometric convex-hull proofs. It has only been scarcely adopted in the literature so far, despite the great flexibility in designing algorithmic proofs for the completeness of polyhedral descriptions that it offers. We suspect that this is partly due to the rather heavy algebraic framework its original statement entails. This is why we present a much more lightweight and accessible approach to Zuckerberg's proof technique, building on ideas by Gupte, Kalinowski, Rigterink and Waterer. We introduce the concept of set characterizations to replace the set-theoretic expressions needed in the original version and to facilitate the construction of algorithmic proof schemes. Along with this, we develop several different strategies to conduct Zuckerberg-type convex-hull proofs. Very importantly, we also show that our concept allows for a significant extension of Zuckerberg's proof technique. While the original method was only applicable to 0/1-polytopes, our extended framework allows to treat arbitrary polyhedra and even general convex sets. We demonstrate this increase in expressive power by characterizing the convex hull of Boolean and bilinear functions over polytopal domains. All results are illustrated with indicative examples to underline the practical usefulness and wide applicability of our framework.

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MS92

A Structural Comparison of Univariate and Bivariate MIP Formulations for Bilinear Problems

We study piecewise linear approximations of the nonconvex variable product $F(x, y) = xy$ over rectangular domains $D = [x^-, x^+][y^-, y^+]$ and their suitability to be presented as a sharp mixed-integer programming (MIP) formulation. We measure the quality of a MIP formulation by two factors, the number of simplices required not to exceed a certain approximation error bound and the tightness of their linear-programming (LP) relaxation. We compare the straightforward approach of using an MIP model for a single bivariate linearization of xy with several univariate approaches that use separable reformulations and approximate univariate functions. For the required number of simplices, we derive upper bounds for the univariate approaches and compare them to a lower bound for the bivariate linearization. We prove that for a small enough approximation error all univariate approaches discussed need less simplices than the direct bivariate linearization. In fact, this advantage of univariate reformulations comes at the cost of poor LP relaxations. While the LP relaxation of the bivariate linearization is equivalent to the convex hull of F over D, the univariate reformulations possess genuinely worse LP relaxations. However, we show that this obstacle can be overcome by additionally reformulating the linear cuts describing the convex hull of F and adding them to the univariate MIP formulations.

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MS92

Convexification of Bilinear and Multilinear Functions

The construction of convex relaxations of non-convex sets is an important ingredient in algorithms for global optimization. In this talk, we focus on the case of sets that can be described by bilinear polynomials. This is relevant, for instance, in blending and pooling problems, and due to the large scale of the problems that have to be solved in practice, there is a strong interest in finding strong relaxations that can be computed efficiently. The combinatorial structure of such a bilinear polynomial can be represented by its co-occurence graph where the vertices correspond to the variables and the edges to products of two variables that occur in the function with a non-zero coefficient. We demonstrate how in some cases the graph structure can be used to derive convex hull characterizations. The proofs make use of an intuitive geometric method proposed by Zuckerberg in 2016. We extend the idea to multilinear functions, where we have to use hypergraphs instead of graphs to represent the structure of the function. In this context we obtain simpler proofs and stronger variants of some recent decomposition results.

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MS92

A Variant of the Boolean Quadric Polytope for the Pooling Problem with Recipes

In this talk, we consider the bipartite Boolean quadric polytope with multiple-choice constraints (BQPMC) and analyse its combinatorial properties. This polytope is of interest when deriving cutting planes for a special variant of the pooling problem, where fixed proportions of the inputs at each pool are given. We present facet-defining inequalities as well separation algorithms for (BQPMC). We also prove complete convex-hull characterizations for certain cases of the polytope based on a proof technique recently introduced by Zuckerberg. Finally, we demonstrate the strength of the facet classes in computational experiments on random as well as real-world pooling instances. It turns out that in many cases we can close the optimality gap almost completely via cutting planes alone, and, consequently, solution times can be reduced significantly.

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MS93

A Non-Smooth Trust-Region Method for Optimization Problems Constrained by Variational Inequalities

We propose a general trust-region method for the minimization of nonsmooth and nonconvex, locally Lipschitz continuous functions that can be applied, e.g., to optimization problems constrained by elliptic variational inequalities. The convergence of the considered algorithm to C- stationary points is verified in an abstract setting and under suitable assumptions on the involved model functions. For a special instance of a variational inequality constrained problem, we are able to properly characterize the Bouligand subdifferential of the reduced cost function, and, based on this characterization result, we construct a computable trust-region model which satisfies all hypotheses of our general convergence analysis. The article concludes with numerical experiments that illustrate the main properties of the proposed algorithm.

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MS93

On the Characterization of Generalized Derivatives for the Solution Operator of the Bilateral Obstacle Problem

We consider optimal control problems for bilateral obstacle problems where the control appears in a possibly nonlinear source term. The non-differentiability of the solution operator poses the main challenge for the application of efficient optimization methods and the characterization of Bouligand generalized derivatives of the solution operator is essential for their theoretical foundation and numerical realization. We derive specific elements of the Bouligand generalized differential if the control operator satisfies natural monotonicity properties. We construct monotone sequences of controls where the solution operator is Gâteaux differentiable and characterize the corresponding limit elements of the Bouligand generalized differential as being solution operators of Dirichlet problems on quasi-open domains which are determined by the respective complements of the active and strictly active sets with respect to the two obstacles. For the reduced objective functional, we obtain two elements of the Clarke subdifferential by using an adjoint formula.

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MS93

Directional Differentiability for Obstacle-Type Quasi-Variational Inequalities via Concavity

We consider the sensitivity analysis of parameterized fixed-point problems that arise in the context of obstacle-type quasi-variational inequalities. Under concavity assumptions we prove that the maximal and minimal elements of the solution set depend Lipschitz continuously on the parameters. Moreover the maximal solution mapping is directionally differentiable and its directional derivatives are the minimal solutions of suitably linearized fixed-point equations. Our approach further the elliptic and parabolic setting simultaneously and also yields Hadamard directional differentiability results in situations in which the solution set of the fixed-point equation is a continuum and a characterization of directional derivatives via linearized auxiliary problems is provably impossible. As illustrative examples, we consider a nonlinear elliptic quasi-variational inequality emerging in impulse control and a parabolic quasi-variational inequality, which involves boundary controls.

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MS94

Exactness Conditions for Semidefinite Relaxation of Nonconvex QCQPS with Forest Structures

In this talk, we propose a new method for checking the exactness of the standard semidefinite relaxation of nonconvex quadratically constrained quadratic programs (QCQPs) whose sparsity can be represented by a forest graph. The check method for nonconvex diagonal QCQPs has already been proposed by investigating the dual problem of the semidefinite relaxation of QCQPs. Our method extends the existing one to forest-structured QCQPs by utilizing perturbated problems and a lower bound for the rank of forest-structured matrices. As applications of our method, we also show some results of exactness including exactness conditions for the semidefinite relaxation of subclasses of QCQPs. The simultaneous tridiagonalization of matrices, which corresponds to the existence of nonsingular matrices that simultaneously tridiagonalizes two or more matrices, permits to consider exactness conditions for more general QCQPs.

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MS94

An Extension of Rooss Improved Version of Chubanovs Method to the Feasibility Problem over the Symmetric Cone

We propose a new variant of Chubanovs algorithm for solving homogenous feasibility problems over a symmetric cone. Our work is inspired by a variant of Chubanovs method proposed in Roos (2018) for linear feasibility problems. Our algorithm (1) finds a vector to determine a tighter upper bound of the sum of eigenvalues of any feasible solution, and (2) using it, decreases the feasible region by rescaling the problem, and then repeat (1) and (2). The generated sequence of upper bounds is reducing by a certain ratio, and the algorithm terminates in a finite number of iterations with the best known computational complexity. We conduct numerical experiments with positive semidefinite cones. The results demonstrate that our method is superior to conventional methods in terms of execution time and accuracy.

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MS94

Efficient SOCP Relaxations for Pooling Problems

We discuss a multi-period pooling problem. The pooling problem is an optimization problem for allocating flow in pipeline network with the minimum cost. When we employ the P-formulation, the pooling problem can be expressed as a nonconvex quadratic-constrained quadratic programming problem, but this problem is known be NP-hard. In this paper, we consider SDP, SOCP and LP relaxations of the pooling problem. In particular, we show that these three conic relaxations provide the same optimal value. In addition, we propose a heuristic method called the rescheduling to find a favorable solution of the pooling problem faster by utilizing the solution from conic relaxations as an initial point and exploiting a mathematical structure of a multi-period problem. Through numerical experiments, we verify that the rescheduling method with SOCP relaxation can significantly improve the computational efficiency.

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MS94

Scenario-Based CVaR Approach for Strategic Decision Support in One-Way Carsharing Systems

As a promising sustainable transportation mean, carsharing is receiving increasing attention around the world. Japan is one of the leading countries in launching the carsharing service. One typical project is the Ha:mo RIDE Toyota, which is a station-based one-way carsharing system. In this study, a scenario-based mean-CVaR model is proposed to optimize the strategic decisions for such systems, mainly including station locations, station capacities and number of vehicles. Based on the limited real trip demand data, different scenario data are generated with Poisson distribution to deal with the data uncertainty and to conduct the experiments. In the results, the efficient frontiers are given to examine the trade-off between return and risk. By using a training and testing method, we also verify whether introducing the risk term has benefits. Additionally, a branch-and-cut algorithm and a scenario decomposition method are applied to solve the proposed model considering the complexity of the problems with plenty of scenarios. Compared with the results from optimization solver, the branch-and-cut method performs favorably in solving small- and medium-scale problems. Furthermore, the scenario decomposition can solve the large-scale problems that cannot be handled by optimization solver or by the branch-and-cut method.

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MS95

Low-Rank PDE-Constrained Optimization with IGA Discretization in Space

Isogeometric analysis (IgA) has become one of the most popular methods for the discretization of PDEs, motivated by the use of nonuniform rational B-splines for geometric representations in industry and science. A crucial challenge lies in the solution of the discretized equations, which we discuss in this talk with a particular focus on PDE-constrained optimization discretized using IgA. The discretization results in a system of large mass and stiffness matrices, which are typically very costly to assemble. To reduce the computation time and storage requirements, low-rank tensor methods have become a promising approach. We present a framework for the assembly of these matrices in low-rank form using tensor train approximations. Furthermore, our framework allows for the exploitation of the resulting low-rank structure of the mass and stiffness matrices, and it can be used to solve a PDE-constrained optimization problem without assembling the actual system matrices and carries the low-rank format over to the solution. We use the block alternating minimal energy method to efficiently solve the corresponding KKT system of the optimization problem. We show several numerical experiments with three-dimensional geometries to demonstrate that the low-rank assembly and solution drastically reduce the memory demands and computing times, depending on the approximation ranks of the domain.

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MS95

Tensor Decompositions for High-Dimensional Hamilton-Jacobi-Bellman Equations

A tensor decomposition approach for the solution of high-dimensional, fully nonlinear Hamilton-Jacobi-Bellman equations arising in optimal feedback control of nonlinear dynamics is presented. The method combines a tensor train approximation for the value function together with a Newton-like iterative method for the solution of the resulting nonlinear system. The tensor approximation leads to a polynomial scaling with respect to the dimension, partially circumventing the curse of dimensionality. A convergence analysis for the linear-quadratic case is presented. For nonlinear dynamics, the effectiveness of the high-dimensional control synthesis method is assessed in the optimal feedback stabilization of the Allen-Cahn and Fokker-Planck equations with a hundred of variables.

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MS95

Tensor Numerical Methods for PDEs Constraint Control Problems with Non-Local and Heterogeneous Operators

Rank-structured tensor approximation of functions and operators by using the traditional canonical (CP), Tucker and tensor train (TT) formats allows the almost linear complexity scaling in dimension. Further data-compression to the logarithmic scale can be achieved by using the method of quantized-TT (QTT) tensor approximation [Boris N. Khoromskij. Tensor Numerical Methods in Scientific Computing. De Gruyter Verlag, Berlin, 2018.]. We discuss the recent results on tensor numerical methods in the optimal control problems constrained by fractional multidimensional elliptic PDEs [G. Heidel, V. Khoromskaia, B. Khoromskij, and V. Schulz. Tensor product method for fast solution of optimal control problems with fractional multidimensional Laplacian in constraints. Journal of Computational Physics, 424, 109865, 2021 and B. Schmitt, B. Khoromskij, V. Khoromskaia, and V. Schulz. Tensor Method for Optimal Control Problems Constrained by Fractional 3D Elliptic Operator with Variable Coefficients. ArXiv:2006.09314, 2020.] focusing on the 3D case. We also sketch the low-rank and tensor approach to periodic/stochastic homogenization problems, which can be adapted to the framework of PDE constraint control problems. The numerical illustrations will be presented. This talk is based on joint works with Volker Schulz, Venera Khoromskaia and Britta Schmitt.

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MS95

Tensor Methods for Optimal Control Problems Constrained by Fractional Elliptic Operators with Variable Coefficients

We introduce tensor numerical methods in order to solve optimal control problems constrained by a fractional elliptic operator with variable coefficients in both 2D and 3D. The equation for the optimal control that arises from the corresponding KKT system is governed by a sum of a fractional elliptic operator and its inverse, $M = A^{\alpha} + A^{-\alpha}$, and is discretized over large spacial grids. Depending on the structure of the variable coefficients and the value of the fractional exponent α, we propose special tailored solution schemes that make use of preconditioned iterative methods. In order to be able to operate on large spacial 3D $n \times n \times n$ grids, we make use of efficient low-rank structures of all involved diagonalizable operators, which induce huge savings concerning the storage and computational complexity. Numerical effects of using different types of preconditioners are presented and discussed.

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MS96

Global Adjoint-Based Shape Sensitivity Analysis

Several scientific computing problems are interested in the sensitivity of a changing surface or boundary on scalar-valued functions approximated by some computational model, e.g. lift and drag of a simulated airfoil or turbine. In the context of parameterizing surfaces and boundaries, active subspaces provide an intuitive change of basis for studying differentiable functions with Euclidean parameter-domain. The active subspace is an eigenspace of the average tensor product of gradients whose basis represents important directions in a domain changing the function more over these directions, on average. These important eigenspaces lead to an explainable and interpretable derivative-based global sensitivity metric. However we seek a global sensitivity analysis of shapes which is independent of a shape-parameterization and subsequently involves reinterpreting the domain as a more general smooth manifold. This reinterpretation, free of a chosen shape-parameterization, necessitates an extension of active subspaces over smooth manifolds. We define ordered geodesics as submanifolds of a Riemannian manifold that change the differentiable function more by an analogous globalizing notion of the average. These important submanifolds become the so-called active manifold-geodesics. We approximate active manifold-geodesics of induced drag over transonic airfoils using a smooth local section of the principal GL-bundle and Stanford's SU2 flow solver with associated adjoint approximations.

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MS96

SEEM: The Smooth Extension Embedding Method

This talk describes a fictitious domain method for the solution of initial boundary value problems in general geometries that admits efficient and straightforward implementations via regular grids. It can be interpreted as a fully discrete meshfree method. The core idea is to reduce the actual problem to a side condition to an optimization problem of a high order norm in an encompassing regular domain/grid.

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MS96

A Fully Discrete Riemannian Approach to PDE-Constrained Shape Optimization

It is well known that there are a number of fundamental differences between continuous and discretized shape optimization problems involving partial differential equations (PDEs). As a consequence, optimization and discretization do not commute. In this talk, we will present an idea for a fully discrete approach to PDE-constrained shape optimization. We explore various ideas to ensure that computational meshes remain non-degenerate throughout the course of the optimization algorithms, building on tools from differential geometry.

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MS97

A Two-Stage Stochastic Variational Inequality Model for Storage and Dynamic Distribution of Medical Supplies in Epidemic

The storage and distribution of medical supplies are important parts of epidemic prevention and control. This paper first proposes a new nonsmooth two-stage stochastic equilibrium model of medical supplies in epidemic. The first stage addresses the storage in pre-disaster phase, and the second stage focuses on the dynamic distribution by enrolling competitions among multiple hospitals over a period of time in post-disaster phase. The uncertainties are the numbers of infected people treated in multiple hospitals during the period of time, which are time-varying around a nominal distribution predicted by historical experience. The two-stage equilibrium model is further approximated and transformed to a monotone two-stage stochastic variational inequality (SVI) model that is computationally tractable, with the aid of a smooth approximation technique. We employ the progressive hedging method (PHM) to solve a case study in the city Wuhan of China suffered from COVID-19 pandemic. Numerical results are presented to demonstrate the effectiveness of the proposed model in planning the storage and dynamic distribution of medical supplies in epidemic.

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MS97

Sparse Solutions of Nonlinear Complementarity Problems

We aim to solve the sparse solutions of the vertical linear complementarity problems. The primal problem is an optimization problem with discontinuous objective function and vertical linear complementarity constraints. To solve this class of discontinuous optimization problem with complementarity constraints, we replace the objective function by a kind of capped folded concave function which is Lipschitz continuous and directional differentiable and show the continuous problem and primal problem have the same global minimizers and optimal value. Then, we utilize relaxation to approximate the complementarity constraints with quadratic constraints. We discuss penalty methods to solve the approximation problem and prove that it is an exact penalty method. By proximal gradient method, we solve the subproblem after smoothing the penalty term. Moreover, we discuss the relationship between parameters and how to select the parameters. In addition, we prove the convergence of the algorithms to a d-stationary point of subproblem and a C-stationary point of the continuous problem. Finally, several applications, e.g., sparse solutions to linear equations, linear complementarity problems, portfolio selection, demonstrate the efficiency of our model to find sparse solutions in practical problems.

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MS97

A Globally and Superlinerly Convergent Projection Semismooth Newton Algorithm for Two-stage Stochastic Variational Inequalities

A projection semismooth Newton algorithm (PSNA) is developed for solving the two-stage stochastic variational inequalities, which is globally convergent and has locally superlinear convergence rate under suitable assumptions. PSNA decomposes the original large-scale problem into a sequence of independent small-scale subproblems to solve in parallel, which is a powerful feature for solving large-scale problems and greatly improves the efficiency of the algorithm. Numerical results for large-scale problems show the efficiency of PSNA.

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MS97

Convergence Analysis of Sample Average Approximation of Stochastic Nonlinear Complementarity Problems: from Two-Stage to Multistage

In this paper, we consider the sample average approximation (SAA) approach for stochastic nonlinear complementarity problems (SNCPs) and study the corresponding convergence properties. We first investigate the convergence of the SAA counterparts of two-stage SNCPs when the first stage problem is continuously differentiable and the second stage problem is locally Lipschitz continuous. After that, we extend the convergence results to a class of multistage SNCPs. Finally, some preliminary numerical tests are presented to illustrate the convergence results.

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MS98

Matrix Optimization Based Euclidean Embedding with Outliers

Euclidean embedding from noisy observations that contain outliers is an important and challenging problem in statistics and machine learning. Many existing methods would struggle with outliers due to a lack of detection ability. In this talk, we propose a matrix optimization based embedding model that can produce reliable embedding and identify the outliers jointly. We show that the estimators obtained by the proposed method satisfy a non-asymptotic risk bound, implying that the model provides a high accuracy estimator with high probability when the order of the sample size is roughly the degree of freedom up to a logarithmic factor. Moreover, we show that under some mild conditions, the proposed model also can identify the outliers without any prior information with high probability. Finally, numerical experiments demonstrate that the matrix optimization-based model can produce configurations of high quality and successfully identify outliers even on large networks.

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MS98

Recursive Importance Sketching for Rank Constrained Least Squares

In this talk, we propose a new Recursive Importance Sketching algorithm for rank constrained least squares optimization (RISRO). As its name suggests, the algorithm is based on a new sketching framework, recursive importance sketching. Several existing algorithms in the literature can be reinterpreted under the new sketching framework and RISRO offers clear advantages over them. RISRO is easy to implement and computationally efficient, where the core procedure in each iteration is only solving a dimension reduced least squares problem. Different from numerous existing algorithms with locally geometric convergence rate, we establish the local quadratic-linear and quadratic rate of convergence for RISRO under some mild conditions. In addition, we discover a deep connection of RISRO to Riemannian manifold optimization on fixed rank matrices. The effectiveness of RISRO is demonstrated in two applications in machine learning and statistics: low-rank matrix trace regression and phase retrieval. Simulation studies demonstrate the superior numerical performance of RISRO.

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MS98

An IEFE-SSNAL for Sparse Parabolic PDE-Constrained Optimization Problems

In this paper, sparse parabolic PDE-constrained optimization problems are considered. The fully discrete finite element approximation method is investigated, in which the time discretization is based on implicit Euler (IE) method, whereas the space discretization is done using the piecewise linear finite element (FE). Some first-order methods have shown efficiency for solving sparse elliptic PDE-constrained optimization problems to a desirable accuracy. However, these methods are not robust with respect to the L^2-regularization parameter. Semismooth Newton (SSN) methods as the high-order methods are the alternative choices in consideration of their locally superlinear convergence. Nevertheless, SSN methods are also sensitive to the L^2-regularization parameter. To overcome this bottleneck, we design a highly efficient and robust IEFE-SSNAL method, where the discretized problem is solved by the semismooth Newton Augmented Lagrangian (SSNAL) method. Global convergence and local linear convergence theory for our method is established. More importantly, we prove that our method is robustness to the L^2-regularization parameter and with respect to the time mesh size τ and the space mesh size h. Numerical results, including the comparison among our approach and several state-of-the-art solvers, are presented to demonstrate the high efficiency and the robustness of our proposed algorithm.

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MS98

An Efficient Proximal Difference-of-Convex Approach for Fitting the Sparse Envelope Model

The sparse envelope model (SEM) is an efficient tool for the parameter estimation and the response variable selection in the multivariate linear regression. However, compared with the nice statistical properties that have been established for the SEM, the study of the algorithmic issues of the SEM is not well-developed. In fact, the computational efficiency of solving the nonsmooth and nonconvex optimization problem arising from the SEM is crucial to the applicability of the SEM, since such a problem should be solved for many times, with different parameters for cross validation, even for fitting only a single instance. In this paper, we propose an efficient difference-of-convex approach for the SEM. We first show how to construct the DC decomposition of the nonconvex optimization problem for fitting the SEM, and then we incorporate the classic DC programming, together with the celebrated accelerated proximal gradient method, to solve the decomposed problem. Extensive numerical experiments are conducted, and the corresponding numerical results suggest that the proposed is far superior to the existing block-wise coordinate descent approach. We have made the algorithm designed in this paper as a Matlab software package, which is publicly available for the potential practitioners.

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MS99

Attouch-Th'era Duality, Generalized Cycles and Gap Vectors

Using Attouch Th'era duality, we study the cycles, gap vectors and fixed point sets of compositions of proximal mappings. Sufficient conditions are given for the existence of cycles and gap vectors. A primal-dual framework provides an exact relationship between the cycles and gap vectors. We also introduce the generalized cycle and gap vectors to tackle the case when the classical ones do not exist.

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MS99

Warped Resolvents: Theory and Applications

Resolvents of set-valued operators play a central role in various branches of mathematics and in particular in the design and the analysis of splitting algorithms for solving monotone inclusions. We propose a generalization of this notion, called warped resolvent, which is constructed with the help of an auxiliary operator. The properties of warped resolvents are investigated and connections are made with existing notions. Abstract weak and strong convergence principles based on warped resolvents are proposed and shown to not only provide a synthetic view of splitting algorithms but to also constitute an effective device to produce new solution methods for challenging inclusion problems. Applications to Nash equilibria and data analysis are discussed.

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MS99

Alternative SOCP Approximations for Polynomial Optimization

In this talk, we consider alternative ways to find strong and efficient conic relaxations for polynomial optimization problems (POP). In particular, we show that second order cone (SOCP) hierarchies can be effectively used to strengthen existing hierarchies of linear programming relaxations for POPs. Specifically, we show that this solution approach is substantially more computationally effective in solving certain POPs for which the more common hierarchies of semidefinite programming relaxations are known to perform poorly. Furthermore, when the feasible set of the POP is compact, these SOCP hierarchies converge to the POPs optimal value.

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MS99

Robust Interior Point Methods for Quantum Key Rate Computation for Quantum Key Distribution

We derive a stable reformulation of the quantum key rate computation for finite dimensional quantum key distribution (QKD) problems. This avoids the difficulties from singularities that arise due to loss of positive definiteness. This allows for the derivation of an efficient Gauss-Newton Interior point approach. Empirical evidence illustrate the strength of this approach as we obtain high accuracy solutions and theoretically guaranteed upper and lower bounds for the quantum key rate.

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MS100

On Starting and Stopping Criteria for Nested Primal-Dual Iterations Encountered in Imaging

The importance of an adequate inner loop starting point (as opposed to an inner loop stopping rule) is discussed for a numerical optimization algorithm consisting of nested primal-dual proximal-gradient iterations. While the number of inner iterations is fixed in advance, convergence of the algorithm is guaranteed by virtue of an inner loop warm-start strategy, showing that inner loop "starting rules" can be just as effective as "stopping rules" for guaranteeing convergence.

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MS100

Inertial Proximal Algorithms for Maximally Monotone Operators

We present a Regularized Inertial Proximal Algorithm to solve convex optimization problems and variational inequalities. It is obtained by means of a convenient finite-difference discretization of a second-order differential equation with vanishing damping, governed by the Yosida regularization of a maximally monotone operator with time-varying index. These systems are the counterpart to accelerated forwardbackward algorithms in the context of maximally monotone operators. A simple example illustrates the behavior of these systems compared with some of their close relatives.

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MS100

Primal-Dual Algorithms for Minimizing the Sum of Three Functions with a Linear Operator

In this talk, I will introduce a new primal-dual algorithm for minimizing f(x) + g(x) + h(Ax), where f, g, and h are convex functions, f is differentiable with a Lipschitz continuous gradient, and A is a bounded linear operator. This new algorithm has the Chambolle-Pock and many other algorithms as special cases. It also enjoys most advantages of existing algorithms for solving the same problem. Then I will present its applications in decentralized consensus optimization.

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MS101

Rank-Constrained Hyperbolic Programming

We extend rank-constrained optimization to general hyperbolic programs (HP) using the notion of matroid rank. For LP and SDP respectively, this reduces to sparsity-constrained LP and rank-constrained SDP that are already well-studied. But for QCQP and SOCP, we obtain new interesting optimization problems. For example, rank-constrained SOCP includes MaxCut and nonconvex QP as special cases, and dropping the rank constraints yield the standard SOCP-relaxations of these problems. We will show (i) how to do rank reduction for SOCP, (ii) that rank-constrained QCQP is polynomial-time solvable, and (iii) an improved result for rank-constrained SDP showing that if the number of constraints is m and the rank constraint is $r = O(m^a)$, then the problem is NP-hard whenever $a < 1/2$. We will also study sparsity-constrained HP and extend results on LP sparsification to SOCP and QCLP. In particular, we show that there always exist (a) a solution to SOCP of cardinality at most twice the number of constraints and (b) a solution to QCLP of cardinality at most the sum of the number of linear constraints and the rank of the matrix in the quadratic constraint; and both (a) and (b) can be found efficiently.

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MS101

Optimization with Sparse Noncommutative Polynomials

Trace polynomials are polynomials in noncommuting variables and traces of their products. While originating in invariant theory, trace polynomials more recently received attention in quantum physics, operator algebra, free probability and quantum information theory. This talk addresses positivity of such polynomials and presents new Positivstellenstze (=algebraic certificates for positivity) in terms of sums of squares and traces of sums of squares. The talk is based on joint works with Victor Magron, James Pascoe, and Jurij Volcic.

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MS101

Exploiting Correlative and Term Sparsity in Noncommutative Polynomial Optimization

This talk focuses on optimization of large-scale polynomials in noncommuting variables, while taking into account correlative and term sparsity in the input data. For correlative sparsity, a converging hierarchy of semidefinite relaxations for eigenvalue and trace optimization is provided. This hierarchy is a noncommutative analogue of results due to Lasserre [SIAM J. Optim. 17(3) (2006), pp. 822–843] and Waki et al. [SIAM J. Optim. 17(1) (2006), pp. 218–242]. The Gelfand-Naimark-Segal (GNS) construction is applied to extract optimizers if flatness and irreducibility conditions are satisfied. Among the main techniques used are amalgamation results from operator algebra. For term sparsity, we provide a new hierarchy of semidefinite programming relaxations, called NCTSSOS. This hierarchy features the exploitation of term sparsity hidden in the input data for eigenvalue and trace optimization problems. We also propose an extension exploiting simultaneously correlative and term sparsity, as done previously in the commutative case. We illustrate the efficiency and scalability of NCTSSOS by solving eigenvalue/trace optimization problems from the literature as well as randomly generated examples involving up to several thousands of variables.

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MS101

The Saddle Point Problem of Polynomials

This paper studies the saddle point problem of polynomials. We give an algorithm for computing saddle points. It is based on solving Lasserre's hierarchy of semidefinite relaxations. Under some genericity assumptions on defining polynomials, we show that: i) if there exists a saddle point, our algorithm can get one by solving a finite number of Lasserre type semidefinite relaxations; ii) if there is no saddle point, our algorithm can detect its nonexistence. The algorithm needs to solve semidefinite programs numerically, so the computed solutions are correct up to numerical errors.

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MS102

Inertial Proximal Block Coordinate Method for a Class of Nonsmooth and Nonconvex Sum-of-Ratios Optimization Problems

In this talk, we consider a class of nonsmooth and nonconvex sum-of-ratios fractional optimization problems with block structure. This model class encompasses a broad spectrum of nonsmooth optimization problems such as the energy efficiency maximization problem and the sparse generalized eigenvalue problem. We first show that these problems can be equivalently reformulated as non-fractional nonsmooth optimization problems and propose an inertial proximal block coordinate method for solving them by exploiting the block structure of the underlying model. The global convergence of our method is guaranteed under the Kurdyka–Lojasiewicz (KL) property and some mild assumptions. We then identify the explicit exponents of the KL property for three important structured fractional optimization problems. In particular, for the sparse generalized eigenvalue problem with either cardinality regularization or sparsity constraint, we show that the KL exponents are 1/2, and so, the proposed method exhibits linear convergence rate. Finally, we illustrate our theoretical results with both analytic and simulated numerical examples.

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MS102

Convergence of Proximal Splitting Algorithms in CAT(k) Spaces

We extend the concept of averaged mappings on linear spaces to almost firm mappings on p-uniformly convex spaces. This includes the analysis of convex combinations and compositions of firm operators. Under the assumption of linear metric subregularity we get linear convergence to fixed points. In the setting of $CAT(\kappa)$ spaces, this gives local linear convergence for common fixed point iterations built from prox mappings (e.g. prox-prox, Krasnoselsky-Mann relaxations, nonlinear projected-gradients).

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MS102

Convergence in Measure of Randomized Algorithms: Beyond the First Moment

We apply a general analysis of fixed point iterations in measure spaces to establish existence of invariant measures and convergence of randomized algorithms for optimization. This both simplifies the analysis of stochastic algorithms in optimization, and opens the door to new Markov Chain Monte Carlo methods. Weaker assumptions than are usually encountered in the analysis of Markov chains guarantee linear/geometric convergence. We present case studies of current interest including stochastic coordinate descents and randomized forward-backward algorithms for large-scale optimization.

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MS102

Numerical Approach to TV Models for Identifying Discontinuous Diffusion Coefficients in Elliptic Equations

Identifying the discontinuous diffusion coefficient in an elliptic equation with observation data is an important nonlinear and ill-posed inverse problem. Models with total variational (TV) regularization have been widely studied for this problem. The resulting TV models are nonconvex and convex if the solution and the gradient of solution are observed, respectively. For the convex case, the theoretically required nonsmoothness property of the TV regularization and the hidden convexity of the models are usually sacrificed by numerical schemes in the literature. For the nonconvex case, it seems there are no efficient algorithms. We will show that the alternating direction method of multipliers can be used to solve these problems and it keeps the desired theoretical properties, but the resulting subproblems are difficult to solve. We will investigate the applications of some optimization techniques and the deep convolutional neural network for these subproblems, and derive some algorithms that are demonstrated to be efficient even for higher-dimensional spaces with fine mesh discretization.

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MS103

Multivariate Convex Regression at Scale

We present new large-scale algorithms for fitting a multivariate convex regression function to n samples in d dimensions—a key problem in shape constrained nonparametric regression with widespread applications in engineering and the applied sciences. The infinite-dimensional learning task can be expressed via a convex quadratic program (QP) with $O(nd)$ decision variables and $O(n^2)$ constraints. While instances with n in the lower thousands can be addressed with current algorithms within reasonable runtimes, solving larger problems (e.g., $n \approx 10^4$ or 10^5) is computationally challenging. To this end, we present an active set type algorithm on the Lagrangian dual (of a perturbation) of the primal QP. For computational scalability, we perform approximate optimization of the reduced subproblems; and propose a variety of randomized augmentation rules for expanding the active set. Although the dual is not strongly convex, we present a novel linear convergence rate of our algorithm on the dual. We demonstrate that our framework can solve instances of the convex regression problem with $n = 10^5$ and $d = 10$—a QP with 10 billion variables—within minutes; and offers significant computational gains (e.g., in terms of memory and runtime) compared to current algorithms.

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MS103

Perturbations and Causality in Gaussian Latent Variable Models

Causal inference is a challenging problem with observational data alone. The task becomes easier when having access to data from perturbing the underlying system, even when happening in a non-randomized way: this is the setting we consider, encompassing also latent confounding variables. To identify causal relations among a collections of covariates and a response variable, existing procedures rely on at least one of the following assumptions: i) the response variable remains unperturbed, ii) the latent variables remain unperturbed, and iii) the latent effects are dense. We examine a perturbation model for interventional data, which can be viewed as a mixed-effects linear structural causal model, over a collection of Gaussian variables that does not satisfy any of these conditions. We propose a maximum-likelihood estimator over the positive definite cone that exploits system-wide invariances to uniquely identify the population causal structure from unspecific perturbation data, and our results carry over to linear structural causal models without requiring Gaussianity. We illustrate the utility of our framework on synthetic data as well as real data involving California reservoirs and protein expressions.

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MS103

Hypothesis Testing over Convex Cones

We consider a compound testing problem within the Gaussian sequence model in which the null and alternative are specified by a pair of closed, convex cones. Such cone testing problems arise in various applications, including detection of treatment effects, trend detection in econometrics, signal detection in radar processing, and shape-constrained inference in non-parametric statistics. We provide a sharp characterization of the GLRT testing radius up to a universal multiplicative constant in terms of the geometric structure of the underlying convex cones. When applied to concrete examples, this result reveals some interesting phenomena that do not arise in the analogous problems of estimation under convex constraints. In particular, in contrast to estimation error, the testing error no longer depends purely on the problem complexity via a volume-based measure (such as metric entropy or Gaussian complexity), other geometric properties of the cones also play an important role. To address the issue of optimality, we prove information-theoretic lower bounds for minimax testing radius again in terms of geometric quantities. Our general theorems are illustrated by examples including the cases of monotone and orthant cones and involve some results of independent interest.

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MS104

Riemannian Stochastic Variance-Reduced Cubic Regularized Newton Method

We propose a stochastic variance-reduced cubic regularized Newton algorithm for the finite-sum problem over Riemannian manifolds. The proposed algorithm requires full gradient and Hessian updates at the beginning of each epoch while it performs stochastic variance-reduced updates in the iterations within each epoch. The iteration complexity of the algorithm to attain an (ϵ, δ)-second order stationary point is shown to be $O(\max\{\epsilon^{-3/2}, \delta^{-3}\})$. Furthermore, the paper proposes a computationally more appealing version of the algorithm which only requires *inexact* solution of the cubic regularized Newton subproblem with the same rate of convergence. Numerical results verify our theoretical findings. The performance of the proposed method is also compared with other second-order optimization algorithms for Riemannian manifolds.

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MS104
Zeroth-Order Riemannian Optimization

We consider stochastic zeroth-order optimization over Riemannian submanifolds embedded in Euclidean space, where the task is to solve Riemannian optimization problem with only noisy objective function evaluations. Towards this, our main contribution is to propose estimators of the Riemannian gradient and Hessian from noisy objective function evaluations, based on a Riemannian version of the Gaussian smoothing technique. The proposed estimators overcome the difficulty of the non-linearity of the manifold constraint and the issues that arise in using Euclidean Gaussian smoothing techniques when the function is defined only over the manifold. We use the proposed estimators to solve Riemannian optimization problems in the following settings for the objective function: (i) stochastic and gradient-Lipschitz (in both nonconvex and geodesic convex settings), (ii) sum of gradient-Lipschitz and non-smooth functions, and (iii) Hessian-Lipschitz. For these settings, we analyze the oracle complexity of our algorithms to obtain appropriately defined notions of e-stationary point or e-approximate local minimizer. Notably, our complexities are independent of the dimension of the ambient Euclidean space and depend only on the intrinsic dimension of the manifold under consideration. We demonstrate the applicability of our algorithms by simulation results and real-world applications on black-box stiffness control for robotics and black-box attacks to neural networks.

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MS104
Riemannian Optimization for Projection Robust Wasserstein Barycenter

Collecting and aggregating information from several probability measures or histograms is a fundamental task in machine learning. One of the popular solution methods for this task is to compute the Barycenter of the probability measures under the Wasserstein metric. However, approximating the Wasserstein Barycenter is numerically challenging because of the curse of dimensionality. In this talk, we propose the projection robust Wasserstein Barycenter (PRWB) that mitigates the curse of dimensionality. This new model projects the probability measures onto a lower dimensional subspace that maximizes the Wasserstein Barycenter objective. The resulting problem is a max-min problem over the Stiefel manifold, which is numerical challenging in practice. Combining the iterative Bregman projection algorithm and Riemannian optimization, we propose two new algorithms for computing the PRWB. The complexity of arithmetic operations of the proposed algorithms for obtaining an ϵ-stationary solution is analyzed. We incorporate the PRWB to a discrete distribution clustering algorithm, and the numerical results on real datasets confirm that our PRWB model helps improve the clustering performance significantly.

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MS104

Robust PCA by Manifold Optimization

Robust PCA is a widely used statistical procedure to recover a underlying low-rank matrix with grossly corrupted observations. This work considers the problem of robust PCA as a nonconvex optimization problem on the manifold of low-rank matrices, and proposes two algorithms (for two versions of retractions) based on manifold optimization. It is shown that, with a proper designed initialization, the proposed algorithms are guaranteed to converge to the underlying low-rank matrix linearly. Compared with a previous work based on the Burer-Monterio decomposition of low-rank matrices, the proposed algorithms reduce the dependence on the conditional number of the underlying low-rank matrix theoretically. Simulations and real data examples confirm the competitive performance of our method.

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MS105

An Algebraic Perspective to Signomial Optimization

Signomials are obtained by generalizing polynomials to allow for arbitrary real exponents. This generalization offers great expressive power, but has historically sacrificed the organizing principle of degree that is central to polynomial optimization theory. We reclaim that principle here through the concept of signomial rings, which we use to derive complete hierarchies of upper and lower bounds for signomial optimization via conditional Sums-of-AM/GM-Exponentials (conditional SAGE). The hierarchy of lower bounds follows by adaptation of the arguments from Wang et al. [arXiv:2003.03731] to the setting of signomial rings, and removes assumptions such as convexity of the feasible set and rationality of signomial exponents. We briefly illustrate the hierarchy by comparison to direct global solvers (e.g., BARON and ANTIGONE) and Moment-SOS relaxations (where appropriate). From there we introduce the hierarchy of upper bounds, and describe a new Riesz-Haviland criterion for signomials that is used to prove completeness of the hierarchy. Throughout the talk we highlight the implications of these techniques for polynomial optimization, both in terms of practical methods and opportunities for future theoretical investigation.

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MS105

An Introduction to SAGE Certificates

Sums-of-AM/GM-Exponentials (SAGE) is a family of decomposition methods for proving function nonnegativity. The bulk of this talk reviews the use of SAGE in global polynomial optimization, its broader applicability to signomials (which may be viewed as generalized polynomials over the positive orthant), and its mathematical lineage. From there we address the essential computational questions: what are the relative entropy programs (REPs) used for computing SAGE certificates? What is known about solving these REPs in practice? And finally, how do REPs differ from geometric programs? In the last part of the talk we review published applications of nonconvex signomial programming and highlight families of unexplored applications where theory suggests SAGE may be effective.

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MS105

A Convex Relaxation Approach for the Optimized Pulse Pattern Problem

Optimized Pulse Patterns (OPPs) are gaining increasing popularity in the power electronics community over the well-studied pulse width modulation due to their inherent ability to provide the switching instances that optimize current harmonic distortions. In particular, the OPP problem minimizes current harmonic distortions under a cardinality constraint on the number of switching instances per fundamental wave period. The OPP problem is, however, nonconvex involving both polynomials and trigonometric functions. In the existing literature, the OPP problem is solved using off-the-shelf solvers with local convergence guarantees. To obtain guarantees of global optimality, we employ and extend techniques from polynomial optimization literature and provide a solution with a global convergence guarantee. Specifically, we propose a polynomial approximation to the OPP problem to then utilize well-studied globally convergent convex relaxation hierarchies, namely, semi-definite programming (SOS hierarchy) and relative entropy relaxations (SAGE hierarchy). Our method exhibits a strong performance for OPP problems up to 50 switching instances per quarter wave utilizing the SAGE hierarchy.

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MS105

A Positivstellensatz for Conditional SAGE

The conditional SAGE certificate has been developed as a sufficient condition for signomial positivity over a convex set and has been shown a promising tool for convex relaxation of signomial and polynomial optimization problems. In this talk, we will discuss a hierarchy for the conditional SAGE certificates, which guarantees that by multiplication of a specific function raised to increasing integer power, successively larger subsets of signomials that are positive over a given convex set may be verified via the conditional SAGE certificate. The hierarchy is shown to be complete assuming compactness of the convex set and rationality of the signomial exponents - multiplication of the function raised to some finite integer can certify all signomials positive over the compact convex set. The completeness theorem is analogous to Reznicks Positivstellensatz in classic algebraic geometry which certifies polynomial positivity with SOS polynomials. The proof of the result rests upon a wonderful extension of the Polya-type Positivstellensatz result due to Dickinson and Povh. Computational experiments including application to parameter learning in machine learning will be discussed.

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MS106

On the Central Path of Semidefinite Optimization: Degree and Worst-Case Convergence Rate

We investigate the complexity of the central path of semidefinite optimization without the strict complementarity condition. We develop an exact algorithm to compute the limit of central solutions, as bounded points in the field of algebraic Puiseux series. As a consequence, we derive an upper bound on the degree of the Zariski closure of the central path and a complexity bound for computing the limit point of the central path. Furthermore, by the application of the quantifier elimination, we provide an upper bound on the worst-case convergence rate of the central path.

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MS106

Alfonso: a Matlab Package for Nonsymmetric Conic Optimization

We present `alfonso`, an open-source Matlab package for solving optimization problems over nonsymmetric convex cones. The software enables optimization over any convex cone as long as a suitable barrier is available for the cone or its dual; this includes hyperbolicity cones and their duals, sum-of-squares polynomials, all semidefinite and second-order cone representable cones, power cones, and the exponential cone. Besides enabling the solution of problems that cannot be cast as symmetric cone programs, it also offers performance advantages for problems whose symmetric cone programming representation requires a large number of auxiliary variables or has a special structure that can be exploited. The worst-case iteration complexity of alfonso is the best known for non-symmetric cone optimization: $O(\sqrt{\nu}\log(1/\epsilon))$ iterations to reach an ϵ-optimal solution, where ν is the barrier parameter of the barrier function of the cone. Alfonso can be interfaced with a Matlab function that computes the Hessian of a barrier function for the cone. A simpler interface is also available to optimize over the direct product of cones for which a barrier has already been built into the code. This interface can be easily extended with new cones. The efficiency of alfonso is shown using problems in which the tailored barrier computation greatly decreases the solution time compared to using state-of-the-art optimization software.

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MS106

How Do Exponential Size Solutions Arise in Semidefinite Programming?

As a classic example of Khachiyan shows, some semidefinite programs (SDPs) have solutions whose size – the number of bits necessary to describe it – is exponential in the size of the input. Exponential size solutions are intriguing, and the main obstacle to solve a long standing open problem: can we decide feasibility of SDPs in polynomial time? Although the consent seems to be that such large size solutions are rare, we prove that they are actually quite common. Precisely, we show that a linear change of variables transforms every strictly feasible SDP into a Khachiyan type SDP, in which the the leading variables have large size. We further show that in SDPs coming from sum-of-squares optimization large variables appear naturally, without any change of variables. Finally, we partially answer the question: how do we represent such large solutions in polynomial space?

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MS107

Locally Positive Semidefinite Matrices

The cone of positive semidefinite matrices plays a prominent role in optimization, and many hard computational problems have well-performing semidefinite relaxations. In practice, enforcing the constraint that a large matrix is positive semidefinite can be expensive. We introduce the cone of k-locally posiitive semidefinite matrices, which consists of matrices all of whose k by k principal minors are positive semidefinite. We consider the distance between the cones of positive and locally positive semidefinite matrices, and possible eigenvalues of locally positive semidefinite matrices. Hyperbolic polynomials play a role in some of the proofs. Joint work with Santanu Dey, Marco Molinaro, Kevin Shu and Shengding Sun.

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MS107

Exact Semidefinite Programming Bounds for Packing Problems

In the first part of the talk, I present how semidefinite programming methods can provide upper bounds for geometric packing problems, such as the kissing number. When these bounds are sharp, they give additional information on optimal configurations, that may lead to prove the uniqueness of such packings. For example, we show that the lattice E8 is the unique solution for the kissing number problem on the hemisphere in dimension 8. However, semidefinite programming solvers provide approximate solutions, and some additional work is required to turn them into an exact solution, giving a certificate that the bound is sharp. In the second part of the talk, I explain how, via our rounding procedure, we can obtain an exact rational solution of a semidefinite program from an approximate solution in floating point given by the solver. This is a joined work with David de Laat and Philippe Moustrou.

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MS107

Dual Nonnegativity Certificates in Polynomial Optimization

We are concerned with the problem of certifying that a given polynomial is nonnegative over a compact set by representing it as a weighted sum of squares (WSOS). In this talk, we develop the theory of dual cone certificates for WSOS-representable polynomials. Whereas previous certificates in the literature are alternate representations of the polynomials they certify, dual certificates are distinct from the certified polynomials; moreover, each dual certificate certifies an entire proper cone of WSOS-representable polynomials. We also present an algorithm for computing the optimal WSOS-lower bound of a given polynomial along with a rational dual certificate, with a linear rate of convergence.

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MS107

Non-SOS Putinar-like Certificates of Non-Negativity: And How to Exploit their Sparsity

A certificate of non-negativity is a way to formulate a given polynomial such that its non-negativity becomes evident. Certificates of non-negativity are fundamental tools for polynomial optimization. Most of the current literature on certificates of non-negativity have been concentrated on certificates based on sum-of-squares (SOS) polynomials. We propose a framework for constructing certificates of non-negativity based on any class of non-negative polynomials satisfying some mild assumptions. These certificates are similarly structured as Putinars certificate. In addition, our framework can be used to obtain sparse certificates of non-negativity which are often much more efficient to compute than non-sparse ones. For instance, we construct sparse certificates based on SDSOS-, SAGE- and SONC-polynomials. We expect our work to close the gap between the applicability of SOS-based and other types of certificates of non-negativity.

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MS108

Cubic Regularization for Conjugate Gradient Methods

This talk will focus on the application of cubic regularization in the context of conjugate gradient minimization (CGM) methods for nonlinear programming. Using Shanno's reformulation of CGM as a memoryless BFGS method, we derive new formulas for the regularized step direction, which can be evaluated without additional computational effort. The new step directions are shown to improve iteration counts and runtimes and reduce the need to restart the CGM.

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MS108

Conjugate Gradient Methods for Machine Learning

Conjugate gradient methods (CGM) and their accelerated variants are widely used in machine learning applications. In this talk, we will focus on the use of cubic regularization to improve the CGM direction for fixed and adaptive learning rates. The approach is similar to Moller's Scaled Conjugate Gradient Method (1990), but the regularization parameter is linked to the learning rate and recalculated in each iteration.

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MS108

A Parallelizable Algorithm for Training Support Vector Machines

We present a parallelizable algorithm for training support vector machines. The algorithm takes advantage of fast projected gradient method, augmented Lagrangian, and a working set selection scheme that allows using a multiprocessor environment to perform computations efficiently. We provide numerical results and discuss some future directions for further development of SVM training.

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MS108

Extension of Piyavskii's Algorithm to Continuous Global Optimization

Not every continuous function is Lipschitz continuous. But, one can (and we will) generalize the definition of Lipschitz continuity to something we'll call ε-Lipschitz continuity and we'll show that a function is ε-Lipschitz continuous if and only if it is uniformly continuous. This connection between Lipschitz and uniform continuity can then be used to extend Piyavskii's algorithm for Lipschitz global optimization over bounded convex sets to the larger domain of continuous global optimization over such sets.

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MS109

A Newton-Type Active Set Method for Nonlinear Optimization with Polyhedral Constraints

A Newton-type active set algorithm for large-scale minimization subject to polyhedral constraints is proposed. The algorithm consists of a gradient projection step, a second-order Newton-type step in the null space of the constraint matrix, and a set of rules for branching between the two steps. We show that the proposed method asymptotically takes the Newton step when the active constraints are linearly independent and a strong second-order sufficient optimality condition holds. We also show that the method has a quadratic rate of convergence under standard conditions. Numerical experiments are presented illustrating the performance of the algorithm on the CUTEst and on a specific class of problems for which finding second-order stationary points is critical.

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MS109

NPASA: An Active-Set Algorithm for Nonlinear Programming

In this talk, we propose a two phase method for solving nonlinear programming problems called the Nonlinear Polyhedral Active Set Algorithm (NPASA) that leverages recent active set methods for polyhedral constrained problems [Hager & Zhang, An Active Set Algorithm for Nonlinear Optimization with Polyhedral Constraints, 2016] to solve general nonlinear programs. The two phase approach is designed to ensure global (phase one) and local (phase two) convergence properties, under reasonable assumptions. We will provide an overview for our algorithm NPASA and present convergence properties for NPASA. In particular, we establish local quadratic convergence of the primal iterates and global error estimator for NPASA and prove that only phase two of NPASA is executed after finitely many iterations.

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MS109

SuiteOPT and the Polyhedral Active Set Algorithm

The talk provides an overview of SuiteOPT, a software package for solving sparse nonlinear optimization problems. A key component of the package is the Polyhedral Active Set Algorithm (PASA). The algorithms, theory, and software will be discussed.

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MS109

Hessian-Based Active-Set Methods for Polyhedral Constrained Optimization

We will talk about an active-set method which uses second-order information to accelerate the convergence for solving polyhedral constrained optimization. This hessian-based active-set method is embedded in the general framework of PASA, a two-phase active set method for polyhedral constrained optimization. Global and local convergence as well as some implementation issues of this hessian-based method will be discussed. Numerical experiments show significant numerical performance improvement over the original gradient-based PASA.

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MS110

First-Order Algorithms for Solving Non-Smooth and Non-Strongly Convex Bi-Level Optimization

Simple bi-level problems are optimization problems in which we seek an optimal solution to an inner problem that minimizes an outer objective function. Such problems appear in many machine learning and signal processing applications as a way to eliminate undesirable solutions. However, since these problems do not satisfy regularity conditions, they are often hard to solve exactly and are usually solved via regularization. Several algorithms were proposed to solve these bi-level problems directly assuming that the outer function is either smooth or strongly convex, and in some cases these methods also provide a rate for obtaining feasibility. In our work, we suggest a new approach that is designed for bi-level problems with simple outer functions, such as the ℓ_1 norm, which are not required to be either smooth or strongly convex. In our new Iterative Approximation and Level-set Expansion (ITALEX) approach, we alternate between expanding the level-set of the outer function and approximately optimizing the inner function over this level- set. ITALEX guarantees that at each iteration of the algorithm the outer objective function is super-optimal, a property that is not known for other bi-level algorithms. We show that optimizing the inner function through first-order methods results in a feasibility convergence rate of O(1/k), which is a rate only shown to be obtained for strongly convex outer functions. We demonstrate this performance through numerical experiments.

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MS110

A Reweighted Penalized Conditional Gradient Method for Nonconvex Penalties

The conditional gradient method (CGM) has been widely used for fast sparse approximation, having a low per iteration computational cost for structured sparse regularizers. We explore the sparsity acquiring properties of a generalized CGM (gCGM), where the constraint is replaced by a penalty function based on a gauge penalty; this can be done without significantly increasing the per-iteration computation, and applies to general notions of sparsity. Without assuming bounded iterates, we show $O(1/t)$ convergence of the function values and gap of gCGM. We couple this with a safe screening rule, and show that at a rate $O(1/(td^2))$, the screened support matches the support at the solution, where $d > 0$ measures how close the problem is to being degenerate. We give some experiments to show the feature selection properties of gCGM under these modified penalties.

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MS110

Analysis of the Frank-Wolfe Method for Convex Composite Optimization Involving a Logarithmically-Homogeneous Barrier

We present and analyze a new generalized Frank-Wolfe method for the composite optimization problem (P) : $\min_{x\in\mathbb{R}^n}\ f(Ax) + h(x)$, where f is a θ-logarithmically-homogeneous self-concordant barrier, A is a linear operator and the function h has bounded domain but is possibly non-smooth. We show that our generalized Frank-Wolfe method requires $O((\delta_0 + \theta + R_h)\ln(\delta_0) + (\theta + R_h)^2/\varepsilon)$ iterations to produce an ε-approximate solution, where δ_0 denotes the initial optimality gap and R_h is the variation of h on its domain. This result establishes certain intrinsic connections between θ-logarithmically homogeneous barriers and the Frank-Wolfe method. When specialized to the D-optimal design problem, we essentially recover the complexity obtained by Khachiyan using the Frank-Wolfe method with exact line-search. We also study the (Fenchel) dual problem of (P), and we show that our new method is equivalent to an adaptive-step-size mirror descent method applied to the dual problem. This enables us to provide iteration complexity bounds for the mirror descent method despite that the dual objective function is non-Lipschitz and has unbounded domain. In addition, we present computational experiments that point to the potential usefulness of our generalized Frank-Wolfe method on Poisson image de-blurring problems with TV regularization.

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MS111

Assessment of Event-Triggered Policies of Nonpharmaceutical Interventions based on Epidemiological Indicators

Nonpharmaceutical interventions have been widely applied around the world to control the current COVID-19 pandemic. Typically, this type of intervention is imposed when an epidemiological indicator in a given population exceeds a certain threshold. Then, the nonpharmaceutical intervention is lifted when the levels of the indicator used have decreased sufficiently. What is the best indicator to use? In this talk, we propose a mathematical framework to try to answer this question. More specifically, the proposed framework permits to assess and compare different event-triggered controls based on epidemiological indicators. Our methodology consists of considering some outcomes that are consequences of the nonpharmaceutical interventions that a decision maker aims to make as low as possible. The peak demand for intensive care units (ICU) and the total number of days in lockdown are examples of such outcomes. If an epidemiological indicator is used to trigger the interventions, there is naturally a trade-off between the outcomes that can be seen as a curve parameterized by the trigger threshold to be used. The computation of these curves for a group of indicators then allows the selection of the best indicator the curve of which dominates the curves of the other indicators. This methodology is illustrated using indicators in the context of COVID-19 using deterministic compartmental models in discrete-time, although the framework can be adapted for a larger class of models.

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MS111

Parameter Estimation for Sars-CoV-2 Models under Uncertainty in the Data

Upon the arrival of the Covid 19, the Research Center for Mathematical Modeling of Ecuador formed a specialized work team to model and simulate the spread of SARS-CoV-2, under various public policy scenarios applied to its containment and with large uncertainty in the official statistics. In this talk we explain the used models and the resulting simulations, and present a Bayesian variational scheme used to estimate the different parameters of the models, in the presence of data uncertainty.

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MS111

Design of Covid-19 Staged Alert Systems to Ensure Healthcare Capacity with Minimal Closures

Community mitigation strategies to combat COVID-19, ranging from healthy hygiene to shelter-in-place orders, exact substantial socioeconomic costs. Judicious implementation and relaxation of restrictions amplify their public health benefits while reducing costs. We derive optimal strategies for toggling between mitigation stages using daily COVID-19 hospital admissions. With public compliance, the policy triggers ensure adequate intensive care unit capacity with high probability while minimizing the duration of strict mitigation measures. In comparison, we show that other sensible COVID-19 staging policies, including France's ICU-based thresholds and a widely adopted indicator for reopening schools and businesses, require overly restrictive measures or trigger strict stages too late to avert catastrophic surges. As cities worldwide face future pandemic waves, our findings provide a robust strategy for tracking COVID-19 hospital admissions as an early indicator of hospital surges and enacting staged measures to ensure integrity of the health system, safety of the health workforce, and public confidence.

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MS111

Robot Dance: Using Optimization for Intervention Against Covid-19 in a Complex Network

Robot Dance is a computational platform developed in response to the coronavirus outbreak, to support the decision making on public policies at a regional level. The tool is suitable for understanding and suggesting levels of intervention needed to contain the spread of diseases when the mobility of inhabitants through a regional network is a concern. Such is the case for Covid-19 that is highly contagious and, therefore, the circulation of people must be considered in the epidemiological compartmental models. Robot Dance anticipates the spread of epidemics in a complex regional network, identifying fragile links where applying differentiated measures of containment, testing, and vaccination are the most effective. Based on stochastic optimization, the model determines optimal strategies on the basis of the commuting of individuals and the situation of hospitals in each district. Uncertainty in the capacity of intensive care beds is handled by a chance-constraint approach. Some functionalities of Robot Dance are illustrated on the state of So Paulo in Brazil, using real data for a region with more than forty million inhabitants.

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MS112

A Fully Adaptive Restarting Level Set Method for Constrained Convex Optimization under Error

Bound Conditions

We propose first-order methods based on a level-set technique for convex constrained optimization that satisfies an error bound condition with unknown growth parameters. The proposed approach solves the original problem by solving a sequence of unconstrained subproblems defined with different level parameters. Different from the existing level-set methods where the subproblems are solved sequentially, our method applies a first-order method to solve each subproblem independently and simultaneously, which can be implemented with either a single or multiple processors. Once the objective value of one subproblem is reduced by a constant factor, a sequential restart is performed to update the level parameters and restart the first-order methods. When the problem is non-smooth, our method finds an ϵ-optimal and ϵ-feasible solution by computing at most $O(\frac{G^{2/d}}{\epsilon^{2-2/d}}\ln^3(\frac{1}{\epsilon}))$ subgradients where $G > 0$ and $d \geq 1$ are the growth rate and the exponent, respectively, in the error bound condition. When the problem is smooth, the complexity is improved to $O(\frac{G^{1/d}}{\epsilon^{1-1/d}}\ln^3(\frac{1}{\epsilon}))$. Our methods do not require knowing G, d and any problem dependent parameters.

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MS112

Optimistic High-Order Methods for Saddle Point Problems

In this talk, we consider solving saddle point problems, and, in particular, we discuss the concept of optimism or negative momentum - a technique which is observed to have superior empirical performance in training GANs. The goal of this talk is to provide a theoretical understanding on why optimism helps, in particular why the Optimistic Gradient Descent Ascent (OGDA) algorithm performs well in practice. To do so, we first consider the classical Proximal Point algorithm which is an implicit algorithm to solve this problem. We then show that OGDA inherently tries to approximate the proximal point method, and this is the rationale behind the negative momentum term in the update of OGDA. We also extend our theoretical results to the case of higher-order methods. In particular, we present higher-order optimistic methods that exploit higher-order information of the function to find a saddle point faster than first-order methods.

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MS112

New Primal-Dual Methods for Minimax Problems Involving (Non)Convex-Linear Coupling Objective Function

In this talk, we will present some recent primal-dual first-order methods for solving minimax problems involving both convex-linear and nonconvex-linear coupling objective functions. Our methods rely on a new combination of different techniques such as smoothing technique, Nesterovs accelerated schemes, randomized coordinate strategy, and variance reduction. We show that our algorithms achieve state-of-the-art convergence rates and oracle complexity under standard assumptions. Our rate can be achieved via either averaging or last iterate sequences. Finally, we show some applications of our results on both synthetic and real datasets.

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MS112

Primal-Dual Methods for Convex-Concave Saddle Point Problems

Saddle point problems have become popular in recent years due to their generality, the versatility of the framework, and wide range of applications in machine learning, game theory, etc. We discuss recent advances in first-order methods for solving such problems. Moreover, we introduce a variance-reduced primal-dual algorithm for solving convex-concave saddle-point problems with the finite-sum structure and nonbilinear coupling function. When the number of component functions is massive, we improve the efficiency of the scheme by periodically computing the full gradient, leading to a progressive variance reduction. We also present the effectiveness of our method by solving a distributionally robust optimization problem.

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MS114

A Derivative-Free Method for Large Scale Nonconvex Nonsmooth Optimization

In this talk, we present results on the approximation of subdifferentials of a broad class of nonsmooth convex and nonconvex functions using the notion of the modified discrete gradients. The new version of the discrete gradient method is introduced to solve large-scale nonsmooth nonconvex optimization problems using their piecewise partial separability. The performance of the proposed method is demonstrated using numerical results on some large-scale academic test problems of nonsmooth optimization.

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MS114

Composite Nonsmooth Optimization

We present a manifold sampling algorithm for minimizing a nonsmooth composition $f = h \circ F$, where we assume h is nonsmooth and may be inexpensively computed in closed form and F is smooth but its Jacobian may not be available. We additionally assume that the composition $h \circ F$ defines a continuous selection. Cluster points of the sequence of iterates generated by the manifold sampling algorithm are shown to be Clarke stationary. We consider the tractability of three particular subproblems generated by the manifold sampling algorithm and the extent to which inexact solutions to these subproblems may be tolerated. Numerical results demonstrate that manifold sampling as a derivative-free algorithm is competitive with state-of-the-art algorithms for nonsmooth optimization that utilize first-order information about f.

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MS114

A Derivative-Free Optimization Approach for Solving Semi-Supervised Clustering Problems

In this talk, a novel model for semi-supervised clustering (SSC) problems with pairwise constraints is introduced. The model is formulated as a nonconvex nonsmooth optimization problem. An auxiliary SSC problem is defined to generate starting points for solving SSC problems. An adaptive SSC (ASSC) algorithm is developed based on a nonsmooth optimization method and an incremental approach to solve these problems. The discrete gradient method is applied to solve the underlying SSC and auxiliary SSC problems. The performance of the ASSC algorithm is evaluated and compared with four benchmarking SSC algorithms on twelve real-world data sets.

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MS115

Probability Maximization via Minkowski Functionals: Convex Representations and Tractable Resolution

We consider maximizing $\mathbb{P}\{\zeta \mid \zeta \in K(x))\}$ over a closed and convex set $\mathcal{X}$. We define $K(x)$ as $K(x) \triangleq \{\zeta \in \mathcal{K} \mid c(x,\zeta) \geq 0\}$ where ζ is uniformly distributed on a convex and compact set $\mathcal{K}$ and $c(x,\zeta)$ is defined as either $c(x,\zeta) \triangleq 1-|\zeta^T x|^m$, $m \geq 0$ (Setting A) or $c(x,\zeta) \triangleq Tx-\zeta$ (Setting B). We show that in either setting,$\mathbb{P}\{\zeta \mid \zeta \in K(x)\}$ can be expressed as the expectation of a suitably defined function $F(x,\xi)$ with respect to an appropriately defined Gaussian density (or its variant), i.e. $\mathbb{E}_{\tilde{p}}[F(x,\xi)]$. Aided by a recent observation in convex analysis, we then develop a convex representation of the original problem requiring the minimization of $g(\mathbb{E}[F(x,\xi)])$ over $\mathcal{X}$ where g is an appropriately defined smooth convex function. We then develop a regularized variance-reduced stochastic approximation (**r-VRSA**) scheme that obviates the need for such unbiasedness by combining iterative regularization with variance-reduction. Notably, (**r-VRSA**) is characterized by both almost-sure convergence guarantees, a convergence rate of $\mathcal{O}(1/k^{1/2-a})$ in expected sub-optimality where $a > 0$, and a sample complexity of $\mathcal{O}(1/\epsilon^{6+\delta})$ where $\delta > 0$.

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MS115

Moment-SOS Hierarchy and Exit Time of Stochastic Processes

The moment sum of squares (moment-SOS) hierarchy produces sequences of upper and lower bounds on functionals of the exit time solution of a polynomial stochastic differential equation with polynomial constraints, at the price of solving semidefinite optimization problems of increasing size. In this note we use standard results from elliptic partial differential equation analysis to prove convergence of the bounds produced by the hierarchy. We also use elementary convex analysis to describe a super- and sub-solution interpretation dual to a linear formulation on occupation measures. The practical relevance of the hierarchy is illustrated with numerical examples. This is joint work with Mauricio Junca and Mauricio Velasco.

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MS115

Efficient Algorithms for Large-Scale Chance Constrained Problems

In this talk, we address large-scale chance-constrained optimization problems where we aim to solve optimization problems under probabilistic nonlinear constraints. Solving such probabilistic nonlinear problems is computationally challenging. Existing methods either provide approximate solutions using sampling-based methods, simplified models, and specific classes of uncertainties such as Gaussian linear problems or deal with small-scale chance-constrained problems. To address chance-constrained problems, we transform the probabilistic optimization problem into a deterministicoptimization problem by replacing the probabilistic constraintswith deterministic constraints. We achieve this by finding an inner approximation of the feasible set of the original probabilistic problem. We provide an analytical approach based on the univariate upper bounds of the indicator functions and higher-order moments of uncertainties to obtain the inner approximation of the chance constraints. The presented analytical method yields a rational polynomial description of the inner approximations and is suitable for large-scale problems with arbitrary probabilistic uncertainties and nonlinear constraints. We compare our method to moment-sum-of-squares optimization-based methods and show that it provides tighter inner approximations. In addition, we show the application of the proposed method in the risk-bounded planning problems of autonomous and robotic systems operating in uncertain environments.

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MS115

On Optimization Problems Involving Probability Constraints: The Logconcave Case

Optimization problems involving probability constraints are notoriously hard to solve numerically, even those known to be convex. More precisely, a direct application of stochastic approximation algorithms to these problems is not possible since probability is an expectation of an indicator function whose gradient is zero almost everywhere. In this talk we present reformulations of of chance constrained optimization problems that overcome this limitation and allow for the application of known stochastic approximation approaches. By leveraging recent results on integrals of level set of positively homogeneous functions, we show that for logconcave symmetric probability distributions, the probability of a set can be recasted as an expectation of a continuous function. This is then exploited to develop efficient algorithms that converge to local optima.

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MT1

AI, Machine Learning and Optimization

See session abstract.

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MT1

AI, Machine Learning and Optimization

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MT2

Quantum Computing and Optimization

See session abstract.

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