

Eigenvalue Analysis and Model Reduction in the Treatment of Disc Brake Squeal

By Volker Mehrmann and Christian Schröder

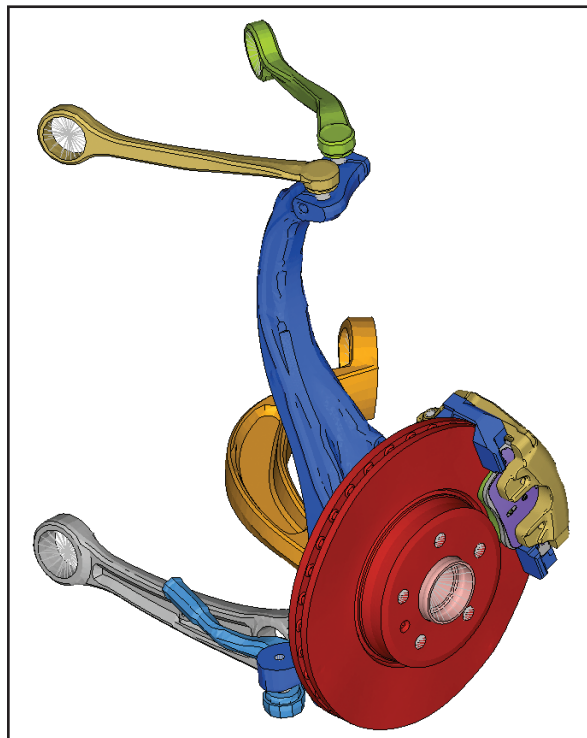


Figure 1a. General view of FE car brake model: industrial model with adjacent components.

Disc brake squeal is a frequent and annoying phenomenon. It arises from self-excited vibrations caused by friction forces at the pad-rotor interface for an industrial brake model [1] (see Figure 1a on the left and 1b on page 3). In order to satisfy customers, the automotive industry has been trying for decades to reduce squeal by changing the design of the brake and the disc. So far, it has found no satisfactory solutions that can be implemented in a systematic way. To improve the situation, several car manufacturers, suppliers, and software companies initiated a joint project, supported by the German Federal Ministry of Economics and Technology, which included two mechanical engineering groups at Technical University (TU) Berlin and TU Hamburg-Harburg, and the numerical analysis group at TU Berlin

[1]. The goal of the project was to develop a mathematical model of a brake system with all effects that may cause squeal, to simulate the brake behavior for many different parameters, and to generate a small-scale reduced-order model that can be used for optimization.

The basic finite element (FE) model for analysis and numerical methods is expressed as the macroscopic equation of motion

$$M_{\Omega} \ddot{u} + D_{\Omega} \dot{u} + K_{\Omega} u = f, \quad (1)$$

where u contains the coordinates (in the FE basis) of the displacements and f is an external force. M_{Ω} , D_{Ω} , and $K_{\Omega} \in \mathbb{R}^{n,n}$ are large, sparse, parameter-dependent coefficient matrices that collect terms proportional to acceleration, velocity, and displacement, respectively. Here M_{Ω} is a positive semi-definite mass matrix. The nonsymmetric matrix D_{Ω} collects damping and gyroscopic effects, and the nonsymmetric matrix K_{Ω} collects stiffness and circulatory effects. The parameter Ω denotes the rotational speed of the brake disc.

Other possible parameters include operating conditions (such as temperature and pad

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Introducing the New SIAM Officers

A new year brings new leadership to SIAM. The SIAM community has elected Nicholas Higham as president-elect, Ilse Ipsen as vice president at large, and Simon Tavener for a third consecutive term as secretary.



President-elect
Nicholas Higham

For full election results, including additions to the Council and Board of Trustees, see page 2.



Leveraging Noise to Control Complex Networks

By Daniel K. Wells, William L. Kath, and Adilson E. Motter

From the diffusion of molecules in a living cell to fluctuations in population levels within an ecosystem, stochasticity pervades our world. When coupled with the inherent nonlinearity of these systems, even small amounts of stochasticity (or “noise”) can generate macroscopic, potentially deleterious outcomes. For example, noise in the expression of genes within a genetic regulatory network can spontaneously change the phenotypes of cancer cells, which might complicate therapeutic strategies targeting particular cell types [4]. Similarly, fluctuations in the populations of key species can propagate throughout a food web, potentially leading to the extinction of other species [5]. Given these far-reaching consequences, it is perhaps surprising that noise has been regarded as little more than a nuisance in the development of methods to control real network systems like those above. Here we take a different approach by illustrating ways through which noise can be accounted for, and in fact exploited, to control network dynamical systems.

A key feature of many network dynamical systems is multistability—the presence of multiple stable states (stable fixed points and/or more general attractors). These states each represent distinct dynamical states that are persistent to small perturbations and in which the system could remain permanently in the absence of noise. In many cases, the noisy dynamics of a nonlinear dynamical system can be modeled as a system of stochastic ordinary differential equations, which in the simplest form is

$$dx = F(x; \Omega) dt + \sqrt{\varepsilon} dW,$$

where Ω are the system parameters and dW is Gaussian noise. The dynamics of this noisy system are actually quite conceptually simple: the system will fluctuate within the basin of a particular attractor for a length of time until suddenly

transitioning to another attractor. When this transition takes place, it will occur in a way that should be intuitive for any hiker—the system is most likely to transition by going through a “mountain pass,” or saddle point that connects the two attractors. Therefore, the dynamics of a noisy, multistable system can be distilled into a continuous time Markov chain \mathbf{R} , where the strength of the noise ε and the heights of the “mountain passes” determine the rates of transition between different stable states. Such a Markov chain approach can capture the dynamics of any noisy multistable system regardless of its dimensionality, and has been applied to model, for example, chemical reactions and the folding dynamics of proteins [7].

What needs to be determined, then, is how to calculate the transition rates between stable states. This question was first considered rigorously for gradient systems (where $\mathbf{F}(x; \Omega) = -\nabla V(x; \Omega)$, for some V), which led to the celebrated Eyring-Kramers law:

$$k_{i,j} \propto \exp[(V(x_i^*; \Omega) - V(z_{i,j}^*; \Omega)) / \varepsilon],$$

where $k_{i,j}$ is the transition rate from attractor x_i^* to attractor x_j^* , and $z_{i,j}^*$ is the location of the highest saddle point on the path separating the two attractors. Determining the rates $k_{i,j}$ either analytically or numerically is the focus of much of the field of transition state theory [3].

The situation is more involved in nongradient systems, where no potential exists. In these systems, the transition rates $k_{i,j}$ between attractors x_i^* and x_j^* can be approximated by employing the Wentzell-Freidlin theory [2], giving

$$k_{i,j} \propto \exp[-S_{i,j}^*(\Omega) / \varepsilon],$$

$$\text{where } S_{i,j}^*(\Omega) = \min_{\phi(t)} \int_{\phi(-\infty)=x_i^*}^{\phi(\infty)=x_j^*} \left\| \frac{d\phi}{dt}(t) - F(\phi(t); \Omega) \right\|^2 dt.$$

Above, $S_{i,j}^*(\Omega)$ is the Wentzell-Freidlin action evaluated along the minimum action path, $\phi^*(t)$. For small noise levels, this path will be the most probable path a noise-induced transition will follow. In general,

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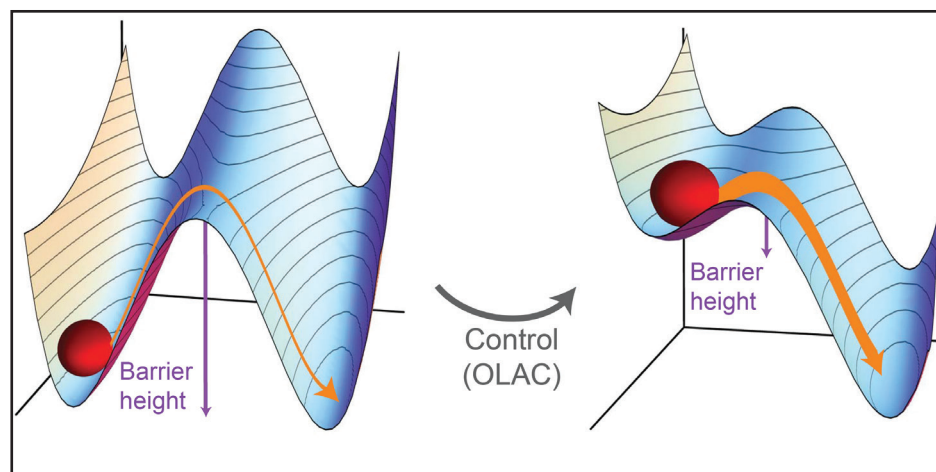


Figure 1. Attractor landscape and control of a network dynamical system. Left: A system initially in the left stable state will eventually undergo a noise-induced transition and will traverse the minimum action path (orange) through the lowest barrier to another attractor. Right: Optimizing the system parameters to lower the barrier height reshapes the landscape topography and substantially increases the probability of the transition.

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6 Machine Learning and the Prospect of a Master Algorithm

Ernest Davis candidly reviews Pedro Domingos' *The Master Algorithm: How the Quest for the Ultimate Learning Machine Will Remake Our World*. The book outlines the techniques of machine learning for a popular audience. Davis applauds Domingos' thorough survey of the major approaches to machine learning but spares no criticism of the book for its inflated goal for machine learning in general, and the master algorithm in particular.

7 RandNLA, Pythons, Oracles, and the CUR to Your Data Problems

Organizers recap the 2015 Gene Golub SIAM Summer School, which took place in Delphi, Greece. From NP-hard problems and matrix factorizations to Delphi's Charioteer statue and the Rio-Antirrio Bridge, the article covers a lot of ground.



8 An Inverted Pendulum: Defying Gravity (and Intuition)

In his recurring column on "Mathematical Curiosities," Mark Levi explains the reasons behind the stability of an inverted pendulum. Look for many more columns to come!

7 Professional Opportunities

New Year Brings New Leadership for SIAM

Members have voted, results are in, and it's time for the SIAM community to meet their newly-elected officers. Those elected will oversee a range of activities, make decisions on behalf of members, and aid in advancing SIAM's mission and goals.

Nicholas Higham, the Richardson Professor of Applied Mathematics at the University of Manchester, is SIAM's 2016 president-elect. On January 1, 2017, he will begin his two-year term as president, succeeding Pam Cook. Higham joined SIAM while working towards his Ph.D., and has been involved with the community for 31 years. He served two terms as vice presi-



Nick Higham, SIAM's 2016 president-elect, will succeed Pam Cook as president in 2017.

dent at large from 2010-2013, and spent eight years on the Board of Trustees and six on the Council. Higham helped establish SIAM Blogs in 2013, has authored four SIAM books, and most recently acted as chair of the SIAM Book Committee. His research interests include numerical analysis, numerical linear algebra, and scientific computing.

Ilse Ipsen will serve a two-year term as vice president at large. She is currently a professor of mathematics and associate director of the Statistical and

Applied Mathematical Sciences Institute at North Carolina State University. Ipsen

was a member of the editorial board for the *SIAM Journal on Matrix Analysis and Applications* from 1997-2014, and has been a member of *SIAM Review's* editorial board since 2004. She spent six years as section editor of *SIAM Review*. Her area of research spans numerical linear algebra, randomized algorithms, and numerical analysis.

Simon Tavener, a professor of mathematics at Colorado State University, was reelected to a third consecutive term as secretary, a position he has held since 2012. Tavener's research interests include numerical analysis and scientific computing, especially error estimation and adaptivity for multi-physics problems, as well as computational biology, including ecology and evolution. He has served as associate dean of Colorado State's College of Natural Sciences since 2011.

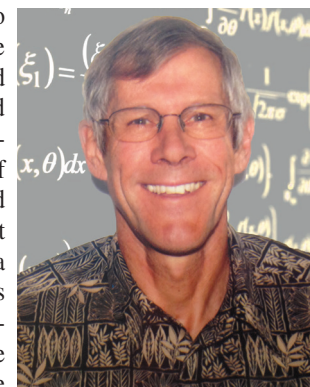
The SIAM community also elected three officers to serve three-year terms on the Board of Trustees. Linda Petzold is currently a computer science professor and director of the Computational Science and Engineering Graduate Emphasis at the University of California, Santa Barbara. She served as SIAM's vice president at large from 2000-2001, and has been a member of the Committee on Science Policy since 2000. Lisa Fauci, associate director of the Center for Computational Science at Tulane University, has been a part of the SIAM Board since 2009. She served as chair of the SIAM Activity Group on Life Sciences from 2009-2011, and spent six years as associate editor of

the *SIAM Journal of Applied Dynamical Systems*. Leslie Greengard is a professor of mathematics and computer science at New York University, as well as director of the Simons Center for Data Analysis at the Simons Foundation. He has organized minisymposia at multiple SIAM annual, CS&E, and ICIAM meetings.

Four members are joining (or rejoining) the Council in 2016, and will serve alongside the remaining council members. Andreas Griewank is the Dean of the School of Information Sciences and Technology at Yachay Tech in Ecuador. Part of the council since 2013, he has authored a SIAM book, is a member of the SIAM Activity Group on Optimization, and helps organize workshops on Automatic and Algorithmic Differentiation. Toby Driscoll of the University of Delaware has been a member of SIAM since 1994. He is a SIAM book author and was associate editor of the *SIAM Journal on Scientific Computing* from 2007-2013. Xiaoye Sherry Li is a senior scientist at the Lawrence Berkeley National Laboratory. She will serve as co-chair for the 2017 SIAM Conference on Computational Science and



Ilse Ipsen is SIAM's new vice president at large.



Simon Tavener was reelected for a third term as secretary.

Engineering, and is currently part of the Gene Golub SIAM Summer School committee. Lastly, Joel Tropp of the California Institute of Technology was the invited speaker for the 2015 Joint Mathematics Meetings. He was also a member of the editorial board for the *SIAM Journal on Matrix Analysis and Applications* from 2013-2015.

SIAM thanks all previous officers for their inspiring work, and looks forward to continued success in the coming year.

Energy Optimization (Rain Is Free, or Isn't It?)

By Claudia Sagastizábal

Readers of *SIAM News* are presumably well aware of the importance of applied mathematics in the advancement of science and industry. Mathematics not only enhances scientific progress, but also hides within simple gestures we instinctively repeat every day. Such is the case when we turn on the lights. What does it take to ensure that every time we enter a dark room and flip the light switch, electricity is available and waiting for us to use?

Sophisticated mathematical optimization tools must be put in place to ensure that we can light our rooms at will. While other

forms of energy—such as gas—can be kept stored until consumed, such storage, at least in amounts that can sufficiently meet the needs of a city, is impossible for electricity. (Batteries do keep power, but at a very small scale). Electricity poses a difficult challenge, as the electrical network should carry power in an amount that is "enough" without being "too much," because any excess is wasted.

Given these constraints, how can one generate electricity in a manner that is both satisfactory for consumers and efficient from the network point of view?

Optimization provides an answer to this question and involves establishing a goal,

called an objective function, to be minimized while respecting certain constraints. The cost of producing electricity, roughly given by the price of burnt coal if energy is generated by a thermal power plant, becomes the objective function. Constraints include several technical rules representing the process of transforming the burnt fuel into megawatts. One



Figure 1. Itaipu, a hydroelectric power plant between Brazil and Paraguay on the Paraná River. Photo credit: International Hydropower Association.

constraint of paramount importance relates to energy demand; ideally, power plants should provide as much electricity as consumers request.

On one side of the issue is the demand constraint, and on the other is the cost of generating the required power. From an energy optimization perspective, estimating consumer demand is a difficult task, one that calls for econometric models and statistical tools. Fortunately, using past consumption records to calibrate a stochastic model makes recurrent events like peak and off-peak hours relatively easy to foresee. Yet even when estimates are conducted from one day to the next, other indeterminate factors – much harder to predict or model – affect electricity demand and consumption. Consider for example an important soccer match, one deciding the outcome of the FIFA World Cup. In Brazil, a large

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Disc Brake Squeal

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pressure) and material properties (friction coefficient, brake geometry and mass distribution, effects of wear, damping, etc.). The excitation of vibrational modes can be investigated by computing the eigenvalues with positive real parts (associated with the unstable behavior of the model) of the quadratic eigenvalue problem associated with (1). This is still a major computational challenge, particularly if solving for many

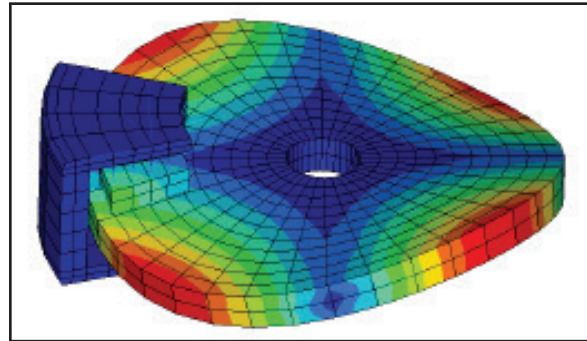


Figure 1b. General view of FE car brake model: simple academic model.

parameter values.

The goal of the project's numerical component was to produce from the large-scale system (1) a small-scale system that can be used for optimizing the original system with respect to parameter variations, and in which the system's complete unstable behavior is present. A particular version of the proper orthogonal decomposition (POD) method was used to generate the reduced-order model. The method computes all eigenvectors associated with right-half-plane eigenvalues for several sample parameter values. This is done by companion linearization and a scaled version of the shift-and-invert Arnoldi method [3] with a tricky shift selection procedure.

The so-called sample matrix is then formed from all these eigenvectors and the equations of motion are projected to the subspace associated with the large singular values of this matrix. This reduces the size of the parametric FE model from one million to about fifty while retaining provably good accuracy for the whole parameter set.

We had access to three FE models: an academic, relatively low-dimensional model, depicted in Figure 1b, which was used to develop the method; and two large-scale models, actually used in industry.

Figure 1a shows one of them. While applying the new technique to the industrial models, we noticed that the eigenvalue computation was severely ill-conditioned; actually, the eigenvalue problem was often close to a singular problem. An analysis of the FE models revealed that they contained highly stiff springs used to avoid rigid connections, a modeling trick that has also been observed in a different context [2]. The negative effects of this technique came as a surprise to the industrial partners, and a similar analysis of other car manufacturers' models demonstrated that this technique is used commonly, although with significant differences in the chosen spring constants.

We devised a sensitivity estimation technique based on pseudo-spectra to automatically detect the presence of these artificial stiff springs and to properly treat the rigid connections associated with the eigenvalue infinity. In combination with effective scaling and shift-and-invert transformations, we implemented and delivered a Python program to the industrial partners. This code will not only be useful in brake squeal studies, but also in other parameter-dependent vibration problems, which have non-proportional damping and other nonsymmetric terms.

To observe the advantage of the new POD method, consider our first (ill-conditioned) industrial model of over 1.2 million degrees of freedom, where the parameter is the scaled rotational speed of the disc. The new method produces better accuracy at

lower reduced dimensions when compared to the traditional modal truncation method, as seen in Figure 2. The traditional modal truncation method uses as projection space the eigenvectors associated with the smallest real eigenvalues of a simplified symmetric and definite linear eigenvalue problem obtained by omitting all damping, gyroscopic, and circulatory terms in (1).

Figure 3 shows a striking example observed for the (very ill-conditioned) second industrial model; the eigenvalue approximations of the two methods are often close together but occasionally noticeably distinct, and sometimes even in different half-planes! In this case the traditional modal truncation method would have missed an eigenvalue that leads to squeal. Moreover, the residuals (indicated by the color of the shown marks (o,+)) of the eigenvalues computed by the traditional method ($\approx 10^{-7}$) are much higher than those by POD ($\approx 10^{-11}$).

In conclusion, the new model reduction method, although more costly, produces much smaller reduced models with an accuracy that is far better than the traditional

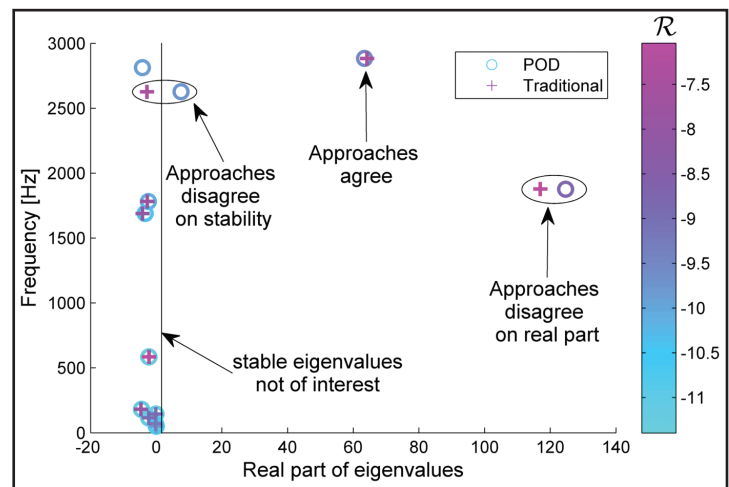


Figure 3. Selected eigenvalues for the two different methods, POD and traditional modal truncation, color coded with their residuals (log scale).

modal truncation method commonly used in industry.

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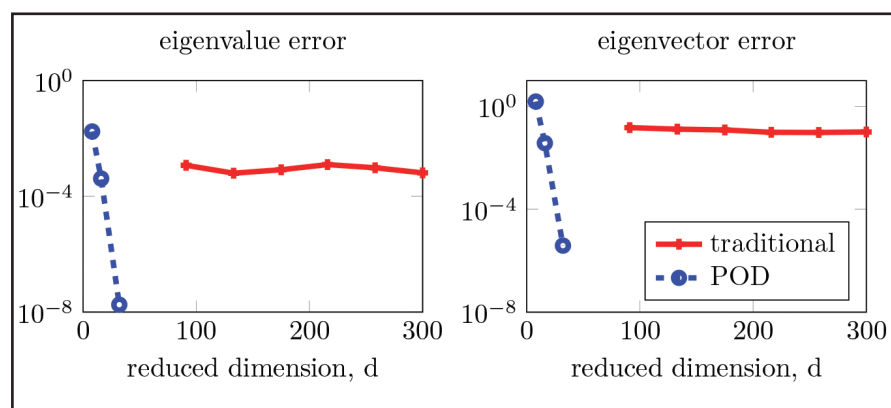


Figure 2. Relation of the various error metrics and the reduced dimension.

Leveraging Noise

Continued from page 1

$S_{i,j}^*$ can only be calculated numerically, but many good algorithms are available to do so [1].

Up to this point we have discussed how network dynamical systems are quite often multistable, how noise can induce transitions between different attractors in these systems, and how the deterministic dynamics $\mathbf{F}(x; \Omega)$ can be employed to calculate the rates of these transitions. Intuitively, then, if we change the system dynamics—by altering the parameters Ω , for example—we can change the transition rates. This, in turn, modifies the dynamics of the Markov chain and could alter its stationary distribution, i.e., the fraction of time spent close to each stable state in the long time limit. What about the inverse problem: how should the tunable parameters of a system be altered to drive the dynamics of our Markov chain to converge to a specific stationary distribution? In particular, we seek to alter the parameters Ω of the noisy dynamical system to reshape the topography of the attractor landscape and thus induce desired transitions, as illustrated schematically in Figure 1 (see page 1).

One way to address this question is by identifying an appropriate objective functional on the space of Markov chains parameterized by Ω , denoted $G(\mathbf{R}(\Omega))$, whose maximum corresponds to the desired stationary distribution of G . This could, for example, be the limiting (long-time) occupancy of a particular stable state of interest.

Looking for parameters that achieve this therefore reduces to another optimization problem, now over the system parameters, of the form

$$\max_{\Omega \in \mathbf{U}} G(\mathbf{R}(\Omega)),$$

where \mathbf{U} denotes the set of possible parameter choices. This problem can be solved numerically using standard algorithms and packages [6]. The combined algorithm, which synthesizes techniques for estimating transition rates between attractors with methods to maximize objective functionals, is termed Optimal Least Action Control (OLAC) [8].

Using OLAC, we can control the response to noise in network dynamical systems with hundreds of variables and thousands of parameters. For example, we have successfully applied this methodology to high-dimensional network models from systems biology and computational neuroscience. One of the lessons we have extracted from these applications is that, when transitions from one stable state to another are optimized, the most likely transition path connecting them often passes through an intermediate stable state. This phenomenon can occur even in systems with a large number of variables, and suggests that “indirect” control strategies—inducing transitions to undesired states as a means to achieve transitions to desired ones—may actually be effective in network dynamical systems.

Other results are also intriguing. For example, when we augmented OLAC with constraints of the form $\sum_i |\Delta\Omega_i| \leq \beta$

known to generate sparsity in many generic optimization scenarios [6], the resulting control interventions often required manipulation of fewer than 10% of all parameters. This suggests that it might be possible to control the response to noise in systems using only a handful of carefully picked parameters, which promises to be especially advantageous in connection with experimental implementations. The question of just how small this set can be for a given control problem remains open.

Ultimately, this work demonstrates that noise, far from being a nuisance, can actually be a tool that allows for the shaping of system dynamics even when other forms of control are not possible. The method we propose as such an approach, OLAC, relies on the fact that a noise-induced transition will typically only follow a single optimal path from one attractor to the other. This observation allows us to reduce the dynamics of an arbitrarily high-dimensional system into a sequence of one-dimensional paths, and in turn into a computationally-tractable, continuous time Markov chain that captures the essence of the dynamics. In general, the study of how to effectively control high-dimensional, noisy, nonlinear dynamical systems (as is common in the case of real network systems) is in its infancy, and this area promises to be an exciting one in years to come.

This article describes results of our recent paper [8], which provides substantially more details about OLAC along with

example applications and relevant references.

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Danny Wells is a graduate student and Bill Kath is a professor of applied mathematics at Northwestern University. Adilson Motter is the Charles E. and Emma H. Morrison Professor of Physics and Astronomy at Northwestern University.

Energy Optimization

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majority of the population will open the refrigerator during half time to get a beer. This action produces a huge spike in energy consumption that the electrical system must face (shutting down power in the middle of the match would be quite unappreciated). This specific type of extreme event happens only once every four years and thus can be addressed by exceptionally over-generating and creating a (larger than usual) reserve of electricity in the network. This reserve, called *spinning reserve*, is also useful should the system face a minor production failure or the breakdown of a line.

An example of a more frequent demand uncertainty relates to temperature. In France, many households have electrical heating. During the winter, if the actual temperature for a given day happens to be even 1°C lower than the forecast predicts, it would require adding the full generation of one nuclear power plant to the system!

The aforementioned examples address coal and nuclear power plants. For environmental reasons, other sources of renewable energy are gaining more weight in the power mix worldwide. Nowadays most power systems include significant percentages of clean technologies that generate electricity from hydraulic and wind-driven sources.

Including renewable energy plants in the optimization problem poses additional challenges related to uncertainty and specific to the distinctive features of each technology. Use of wind energy demands a model defined by historical records that applies econometric techniques to estimate the wind at any given hour of the day. Water is a completely different matter, especially when the hydraulic energy is generated by a plant with a reservoir (the generation of run-of-the-river plants is modeled similarly to wind power). In fact, in terms of energy optimization a hydro-reservoir is a (smart!) way of storing large amounts of energy. Stored water is the equivalent of stored power. Water is the fuel needed to produce hydraulic energy; just letting the water run

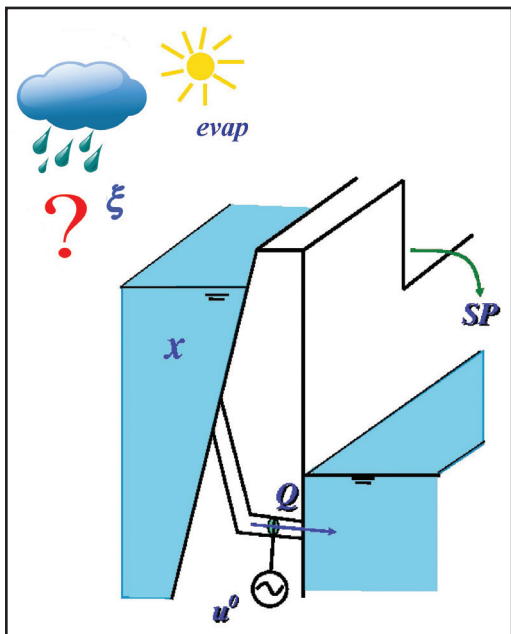


Figure 2. The reservoir volume x decreases due to evaporation and to water released, either by spillage SP or passing through the turbines Q , to generate power u^p . The stored volume of water can increase with the inflows ξ , which are unknown.

through the turbines makes the power available to the system. In this case, uncertainty comes from the reservoir volumes, which in turn depend on the pluvial regime and the amount of melted snow. Once again, proper econometric models must be found to estimate the water inflows on the basis of past data.

The impact of inflow uncertainty in hydrogeneration is very different from other kinds of energy generation. As long as the hydro plant has a reservoir, the volume of

available water can be considered known from one day to the next; contrary to wind power, there is no uncertainty in this data. Uncertainty is instead in the production cost: how much does it cost to generate hydropower? If we consider the fuel price, like with thermal plants, hydroelectricity costs nothing; water is free!

Here arises a curious phenomenon, resulting from the model itself and not from the data. We can refer to it as the “end-of-the-world” effect. Consider a simple setting with only two power plants: one thermal and one hydro plant with a reservoir. Generating thermal power is expensive due to the coal price, while hydropower costs nothing. Since the optimization problem attempts to minimize cost, its solution will fatally deplete the reservoir whilst trying to generate as much hydraulic power as possible. This solution may very well be the best one for the optimization problem, but



Figure 3. Wind turbines harness clean energy from wind and convert it to electricity.

it is certainly not desirable in the long term. The optimization problem is short-sighted and does not realize it can be problematic if, after its decision horizon, there is no more water in the reservoir.

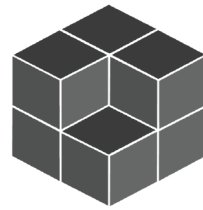
A mathematical optimization formulation addresses the “end-of-the-world” effect. The formula operates on the following key observation: for power generation purposes, a water reservoir is nothing but an electricity storage. Water is dormant energy and, as such, can be priced by computing its cost of substitution. Specifically, if we generate hydroelectricity to save money today, the reservoir level will go down. Then, if there is a drought in the future, we may have to burn (expensive) coal because the reservoir was never refilled. We can use the cost of generating this type of “emergency” thermal power to price the future cost of water.

In mathematical optimization terms, those calculations amount to the approximate computation of the value function of a multistage stochastic linear program. This is by no means an easy task, because often such linear programs are simply intractable. For the Brazilian power system, for example, the linear programming problem must consider 20^{119} possible scenarios for uncertainty. Only by suitably combining decomposition and sampling methods is it possible to define lower and upper bounds that sandwich the future cost function up to some confidence level. Thanks to this sophisticated machinery, the future cost of water can replace the zero cost for hydrogeneration in the optimization problem. The new objective function will prevent reservoirs from experiencing depletion at the end of the decision horizon. This strategy makes it possible for us to get power when we turn on the lights.

It should also prevent unwelcome blackouts during massively popular events like the Super Bowl or the next FIFA World Cup final.

This article is based, in part, on Claudia Sagastizábal’s invited lecture at the 8th International Congress on Industrial and Applied Mathematics (ICIAM) held in Beijing, China, in August 2015.

Claudia Sagastizábal is a visiting researcher at the Instituto Nacional de Matemática Pura e Aplicada in Rio de Janeiro, Brazil.



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Symposium Connects Government Problems with State-of-the-Art Network Science Research

By *Rajmonda S. Caceres and Benjamin A. Miller*

In the last several years, network science has grown significantly as a field at the intersection of mathematics, computer science, social science, and engineering. Topics of interest include modeling and analysis of network phenomena, large-scale computation and data management, models for information and epidemic spreading through networks, and inference of information about entities based on observable connections. While basic research focuses on developing understanding in each of these areas, the ultimate goal in a practical setting is to use this understanding to achieve some application-specific objective.

In diverse mission areas, such as cyber security, counterterrorism/counterinsurgency, air traffic control, and bioengineering, the data of interest are inherently interconnected. Using a network or graph representation for the data allows for an additional level of insight not available when considering the data independently.

In 2010, as part of a research effort funded by the Office of Naval Research, staff at Massachusetts Institute of Technology's Lincoln Laboratory in Lexington, Massachusetts, a Federally Funded Research and Development Center (FFRDC) for the United States Department of Defense, set out to build a community of interest through a symposium specifically focused on exploitation of graph data. The goal was to bring together academic researchers, industry practitioners, and end users to discuss problems of interest to the U.S. Government, and match these with the state-of-the-art models and techniques developed in the network science research community. Since its inception, the Graph Exploitation Symposium (GraphEx) has been held annually as a meeting to facilitate this interaction.

The following themes outline the current research frontier within the network science field, much of which was in evidence at the sixth annual GraphEx Symposium,¹ held last July in Dedham, Massachusetts.

Controllability of large-scale, complex networks: Many human-engineered systems—including computational infrastructures, transportation systems, and electrical power grids—behave like large-scale, complex networks with different layers and components interacting in non-trivial ways. The susceptibility of such systems to local shocks is amplified by network cascading effects. Researchers currently lack the ability to quantify vulnerability and resilience of large-scale, complex networks at the system level. Symposium speakers at GraphEx 2015 put forward several suggestions to address this important challenge:

- Combine network science approaches with existing rich methodologies from the fields of control theory and decision theory to model dynamically changing demands on the engineered complex system.
- Rigorously measure, model, and assess the system architecture at different levels and under different constraints and disruptions.
- Design complex systems that are dynamic and stable by adaptively allocating resources/services through closed-loop feedback channels (e.g. software-defined wireless networks and intelligent transportation systems).
- Design complex network control mechanisms that can robustly handle stochastic cascades on the network while also localizing control effects.

User-centric algorithms: A number of talks addressed the concept of combining user-centric, private, rich data with

global, incomplete, publically-available data, in ways ranging from estimating systemic risk in transportation networks to designing recommender systems on social networks. Mathematical models and algorithms that can handle a seamless and efficient integration of the two data regimes have implications beyond accuracy improvements on inference tasks. Such models have the potential to become enabling technologies as society enters the new era of data democratization and user self-awareness and empowerment.

Noise and interference in networks: Exploiting graphs in the presence of noise and interference is another recent topic of interest in the community, and several presentations touched on this point. In practice, users typically have some prior knowledge (or domain expertise) that suggests probable structure within the network, and algorithms should be developed in consideration of the fact that some of the structure is uninteresting. The symposium included discussions about experimental design in the presence of interference in order to optimize inference ability from the measurements. As community detection relies on metrics that are sensitive to noise in the data, metrics that are resilient to noisy observations was another topic of interest.

Adversarial network analysis: Adversarial interference is an important special case in noisy graph analysis. In this setting, an adversary specifically manipulates the data to counter and misdirect the exploitation task. This area has significant implications for tasks in cyber security and counterterrorism, when a common objective is to uncover a subgraph of interest in which actors are deliberately covert. Presentations on this topic included models for attacker behavior and classes of methods to mitigate the effects of purposeful data corruption.

Multi-modal, multi-layer networks: Since networks change over time and have different connections when seen through different media, analyzing dynamic graphs and multigraphs has become a necessity. Multiple presentations addressed fusion of information over time and across multiple observations. Challenges identified in this area include development of models for temporal evolution of graphs, optimal fusion of information across modalities, and quantification of the benefits and limitations of inference across observations.

Big data analysis and management: Graphs are frequently extracted from extremely large datasets, and dealing with data of this scale

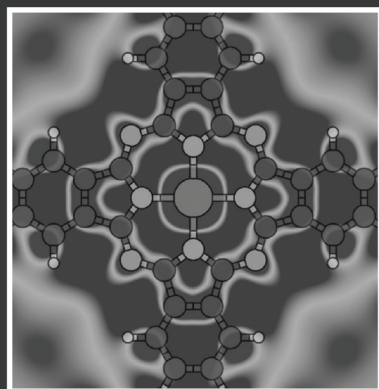
and variety is a challenge inherent in modern network analysis. In this context, the symposium included presentations on personalized recommendations from global data and exploitation of open source and social media data for disaster response. From the perspective of big data management, there are currently active efforts toward native implementation of key computational kernels for graph exploitation algorithms in a large-scale database system.

Bringing together unique perspectives from research, applications, and operations, the sixth annual GraphEx Symposium helped influence the direction of basic network science research in support of current critical technological needs. As capabilities and technologies evolve, the symposium organizers intend to maintain GraphEx as a venue for ensuring continued research-to-practice connectivity.

This work is sponsored by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract FA8721-05-C-0002. Opinions, interpretations, conclusions, and recommendations are those of the authors and are not necessarily endorsed by the United States Government.

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INSTITUTE FOR PURE AND APPLIED MATHEMATICS



Understanding Many-Particle Systems with Machine Learning

September 12 – December 16, 2016 | Los Angeles

Organizers: **Alán Aspuru-Guzik** (Harvard University), **Gabor Csanyi** (University of Cambridge), **Mauro Maggioni** (Duke University), **Stéphane Mallat** (École Normale Supérieure), **Marina Meila** (University of Washington), **Klaus-Robert Müller** (Technische Universität Berlin), and **Alexandre Tkatchenko** (Fritz-Haber-Institut der Max-Planck-Gesellschaft).

SCIENTIFIC OVERVIEW

Interactions between many constituent particles (bodies) generally give rise to collective or emergent phenomena in matter. Even when the interactions between the particles are well defined and the governing equations of the system are understood (for example the Coulomb interaction between protons and electrons and the Dirac/Schrödinger equation in quantum mechanics), the collective behavior of the system as a whole does not trivially emerge from these equations. Examples of collective behavior are abundant in nature, manifesting themselves at all scales of matter, ranging from atoms to galaxies. Machine learning methods have been used extensively in a wide variety of fields ranging from, for example, the neurosciences, genetics, multimedia search to drug discovery. Machine learning models can be thought of as universal approximators that learn a (possibly very complex) nonlinear mapping between input data (descriptor) and an output signal (observation).

It is the goal of this IPAM long program to bring together experts in many particle problems in condensed-matter physics, materials, chemistry, and protein folding, together with experts in mathematics and computer science to synergetically address the problem of tackling emergent behavior and understanding the underlying collective variables in many particle systems.

WORKSHOP SCHEDULE

- Understanding Many-Particle Systems with Machine Learning Opening Day: September 12, 2016
- Understanding Many-Particle Systems with Machine Learning Tutorials: September 13-16, 2016
- Workshop I: Machine Learning Meets Many-Particle Problems: September 26-30, 2016
- Workshop II: Collective Variables in Classical Mechanics: October 24-28, 2016
- Workshop III: Collective Variables in Quantum Mechanics: November 14-18, 2016
- Workshop IV: Synergies between Machine Learning and Physical Models: December 5-9, 2016
- Culminating Workshop at Lake Arrowhead Conference Center: December 11-16, 2016

PARTICIPATION

This long program will involve senior and junior researchers from several communities relevant to this program. You may apply for financial support to participate in the entire fourteen-week program, or a portion of it. We prefer participants who stay for the entire program. Applications will be accepted through **June 12, 2016**, but offers may be made up to one year before the start date. We urge you to apply early. Mathematicians and scientists at all levels who are interested in this area of research are encouraged to apply for funding. Supporting the careers of women and minority researchers is an important component of IPAM's mission and we welcome their applications. More information and an application is available online.

www.ipam.ucla.edu/mps2016



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¹ Information about Lincoln Laboratory's Graph Exploitation Symposium, including proceedings of past meetings, can be found at <https://events.ll.mit.edu/graphex/>.

Machine Learning and the Prospect of a Master Algorithm

The Master Algorithm: How the Quest for the Ultimate Learning Machine Will Remake Our World. By Pedro Domingos, Basic Books, New York, 2015, 352 pages, \$29.99.

Machine learning (ML) has suddenly become very hot. It feels like every week, a machine learning algorithm achieves a major advance in some exciting application; and every other day the popular media publishes exaggerated accounts of these advances, or breathless predictions of what the future has in store. Over the last thirty-five years, ML has gone from being a largely-abandoned niche area of artificial intelligence to a central paradigm within computer science. Machine learning completely dominates applications such as computer vision, speech understanding, and recommender systems in addition to all forms of natural language processing.

Pedro Domingos' book, *The Master Algorithm*, presents an introduction to the techniques of ML, written for a popular audience. It seems to be the first popular book on ML, so it is certainly an important contribution toward general understanding of this enormously important technology.

Chapters 3-7 of Domingos' book survey the five major approaches to supervised ML: symbolic, connectionist, evolutionary, probabilistic, and exemplar-based. Chapter 8 covers unsupervised learning and meta-learning.

These chapters are well-written, clear, and balanced; Domingos carefully describes the intuitions behind each approach, the practical successes the approach has attained, its strengths, and its inherent weaknesses. The true believers in each of the approaches will undoubtedly complain that Domingos short-changed their own approach and handled the other approaches much too politely. The author gives very clear accounts of overfitting and of "the curse of dimensionality," the two great hazards of ML. He almost entirely avoids the use of mathematics.

At his best, Domingos can be extremely good. He offers sharp, insightful statements of points easily overlooked. For instance, he writes that, **"The most important thing about an equation is all the quantities that don't appear in it; once we know what the essentials are, figuring out how they depend on each other is often the easier part."** Overall, these six chapters are a fine introduction to the state of the art of ML.

If only Domingos had been content with that! Unfortunately he has other things in mind, and these seriously degrade the book's overall quality. I found the prologue and chapters 1 and 2 so uncongenial that I almost didn't make it to chapter 3, and my objections

returned in full force upon reaching chapters 9 and 10.

In addition to explaining the actual state of the art, Domingos has two additional goals. The first, explicit in the book's title, is to develop the idea of a "Master Algorithm" for machine learning, which will subsume all other forms of learning and be able to learn

anything that can be learned, and to argue that Domingos' own "Alchemy" system is a major step in that direction.

The second objective, implicit but pervasive and very conspicuous, is to hype the present accomplishments and future impacts of ML as raucously as possible. In pursuit of this goal, the book is generally overwrought, sometimes seriously misleading or simply wrong, and occasionally really quite strange.

For example, in presenting connectionist models, Domingos gets carried away with phase transitions and the idea of an S-curve, which he characteristically calls "the most important curve in the world." He spends an entire page enumerating S-curves and phase transitions, including some very doubtful examples. Paradigm shifts in science and the fall of empires are supposedly S-curves. Falling in love, getting a job, and losing a job are allegedly phase transitions;

clearly at this point "phase transition" just translates to "important change."

Domingos' view of computerization's past impact on science is wildly exaggerated. He writes that **"If computers hadn't been invented, science would have ground to a halt in the second half of the twentieth century."** It certainly would have been impeded, and some discoveries would have been impossible, but it seems safe to say that only a small fraction of scientific discoveries before about 1990 relied critically on computers.

Moreover, Domingos' view of the future impact of the Master Algorithm is fantasy: **"Science today is thoroughly balkanized, a Tower of Babel where each subcommunity can see only into a few adjacent subcommunities."** He then proceeds to state that the Master Algorithm would offer a unified perspective of all science, one that could even lead to a new theory of everything. Even if a Master Algorithm could derive each scientific theory from data, there is no reason to expect that it would provide a unifying view, rather than a collection of separate theories. Domingos continues by saying that **"The Master Algorithm is the germ of every theory: all we need to add to it to obtain theory X is the minimum amount of data required to induce it. (In the case of physics, that would be the results of perhaps a few hundred key experiments)."** That estimate is certainly too low by at least a factor of one hundred.

In chapter 10, Domingos presents his vision of the future. Some aspects of this seem reasonable; in particular, I agree with his belief that there is no danger of computers developing their own goals à la Skynet and exterminating or enslaving us. Other thoughts, however, appear both weird and dreary, like the following Baudrillardesque nightmare: **"In this rapidly approaching future, you're not going to be the only one with a 'digital half' doing your bidding twenty-four hours a day. Everyone will have a detailed model of him- or herself, and these models will talk to each other all the time."** He proceeds to give examples for how this will happen: **"If company X is looking to hire, its model will interview your model. It will be a lot like a real, flesh-and-blood interview . . . but it will take only a fraction of a second . . . Same with dating."**¹

Domingos does not explain why a company would trust that your avatar is an accurate portrayal of yourself, nor why the company should not hire the avatar instead, since it presumably does the same things thousands of times faster.

The issue most important to Domingos is his Master Algorithm conjecture: **"All knowledge — past, present, and future — can be derived from data by a single, universal learning algorithm."**

In chapter 2, he presents many different arguments for the hypothesis, drawing evidence from fields such as neuroscience, evolution, physics, statistics, and computer science.

In my opinion, these assertions are incoherent. The different arguments rely on varied interpretations of the terms "data," "single," "universal," "learning," and "algorithm," and therefore point in different directions. For instance, Domingos bases his case for the neuroscience perspective on the uniform structure of the cortex. Yet in chapter 9, he is willing to consider a Master Algorithm which calls on a variety of very different algorithms and combines their votes. The uniform

See *Master Algorithm* on page 7

¹ Felicia Day's "Do you wanna date my avatar?" (2009) is a particularly insightful discussion of this issue: <https://www.youtube.com/watch?v=urNyg1ftMIU>.

BOOK REVIEW

By Ernest Davis

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Master Algorithm

Continued from page 6

structure of the cortex is, if anything, evidence against a Master Algorithm of this kind. The kind of algorithm he proposes would be consistent with a brain that combines pieces of very diverse structures.

As Domingos himself observes, the Master Algorithm is very unlike existing trends in machine learning, which generally involve highly-handcrafted algorithms for fairly narrowly-defined tasks. Indeed, it is unlike anything that we have seen in computer science. Domingos' argument from the computer science viewpoint rests on the fact that the many NP-complete problems are, in a certain sense, actually the same problem. However, it seems to me that this points in exactly the opposite direction. NP-complete problems are all reducible to the problem of Boolean satisfiability, but there are, probably, tens of thousands of different algorithms for solving specific NP-complete problems, depending on the specifics of the problem and on the desired features of the solution and the algorithm.

The *Master Algorithm* does a fine job of explaining machine learning techniques to the general public. Unfortunately, it is also often extremely misleading. If you have a lay friend who wants to understand ML, by all means recommend it, but do so with a warning.

Ernest Davis is a professor of computer science at the Courant Institute of Mathematical Sciences, NYU.

RandNLA, Pythons, and the CUR for Your Data Problems

By Efstratios Gallopoulos, Petros Drineas, Ilse Ipsen, and Michael W. Mahoney

A few dozen graduate students and Ph.D. candidates, selected from a pool of over 140 highly-qualified applicants from prestigious universities around the world, attended the 2015 Gene Golub SIAM Summer School¹ (G2S3 2015) in Delphi, Greece, last summer. Co-organizers Ilse Ipsen (North Carolina State University), Petros Drineas (Rensselaer Polytechnic Institute), Michael Mahoney (University of California, Berkeley), and Stratis Gallopoulos (University of Patras) served as instructors along with Ken Clarkson (IBM Research-Almaden).

The theme of this year's school, Randomized Numerical Linear Algebra (RandNLA), is an interdisciplinary research area that exploits randomness as an algorithmic resource for the development of improved matrix algorithms for ubiquitous problems in large-scale data analysis. It utilizes ideas from theoretical computer science, numerical linear algebra, high-performance computing, and machine learning and statistics to develop, analyze, implement, and apply novel matrix algorithms. These algorithms can then facilitate the manipulation and analysis of so-called big data in numerous areas. Many popular machine learning

¹ <http://scgroup19.ceid.upatras.gr/g2s32015/>

...Reporting from G2S3 2015 in Delphi

and data analysis computations can be formulated as problems in linear algebra, but the questions of interest in machine learning and data analysis applications are very different from those historically considered in numerical linear algebra.

For instance, NP-hard problems have made their way into numerical linear algebra, a significant paradigm shift for numerical analysts who have traditionally formulated their problems to be solvable in polynomial time. As an example, most formulations of the Column Subset Selection problem are intractable, as are most formulations of the so-called Non-negative Matrix Factorization (NMF) problem. Alternatively, matrix factorizations—if properly instructed—can be used to discover latent information in the data, thus providing qualitative insight and interpretability, which is often of interest in scientific data applications. In this case, CUR is a natural factorization that provides a low-rank approximation of the underlying matrix using a product of selected Columns C and Rows R with a possible middle factor U (a tri-factorization). When the problem is massive in size and a CUR

decomposition is sought, randomization becomes essential. More generally, random sampling and projection methods allow one to design provably accurate algorithms for problems containing the following: matrices so large that they require novel models of data access; matrices that cannot be stored at all, or can only be stored in slow-memory devices or only accessed via oracle calls; and/or problems that are computationally expensive or NP-hard. Randomized CUR and other low-rank decompositions lead to tractable solutions for terabyte-sized data, and have

See **RandNLA** on page 8



Attendees listening attentively to the lectures. Forefront: (left to right) graduate students Hyunghoon Cho (MIT) and Michael Hynes (Waterloo).

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An Inverted Pendulum: Defying Gravity (and Intuition)

If the pivot of the pendulum (Figure 1) is vibrated vertically with a sufficiently high frequency, then the pendulum becomes stable in its upside-down position. This striking phenomenon, discovered and demonstrated by Stephenson in 1908

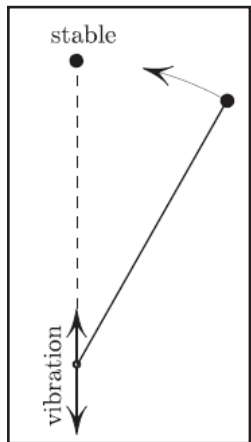


Figure 1. The pendulum is a point mass on a massless rigid rod.

Wishing to observe the Kapitza effect directly, I had originally planned to build a device to vibrate the pivot but fortunately realized, before spending time and money, that I have this device at home. The resulting demonstration can be seen online at <https://www.youtube.com/watch?v=CHTibqThCTU>.

The inverted pendulum was V.I. Arnold's favorite demonstration; he used an electric shaver which has a reciprocating arm inside.

Standard explanations via averaging theory, or by computation of special cases such as in [1], are not intuitive. Here instead is a geometrical/intuitive explanation. In a nutshell, stability is due to the centrifugal force

of a non-existent constraint, as explained below.

Figure 2 shows the pivot oscillating between two points (the amplitude is greatly exaggerated in this figure). We assume that the pivot's acceleration is very large (thus so is the frequency); this means that the rod is under great tension or compression for most of the period. This great force acting upon the bob is aligned with the direction of the rod. As the leading order approximation, we assume that the bob actually moves

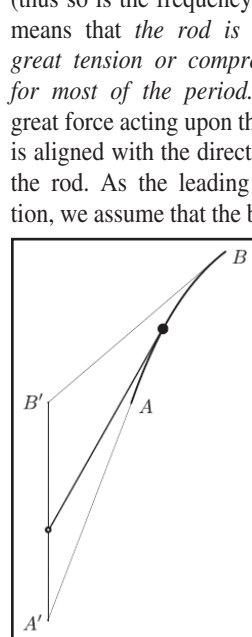


Figure 2. The leading order approximation of the motion.

in the direction of this force. This assumption forces the bob to travel in an arc AB of a tractrix, i.e. the pursuit curve.¹ To summarize, we constrained the bob to an arc AB. This constraint is somewhat innocent since it does not interfere with the huge push-pull force of the rod acting on the bob. Now the mass constrained to the curve pushes with a centrifugal force mkv^2 against the constraint, Figure 4; here k is the curvature of the tractrix. This push is towards the top, suggesting that the top

¹ The tractrix is defined by the property that all the tangent segments connecting it to a straight line have the same length, Figure 3.

MATHEMATICAL CURIOSITIES

By Mark Levi

equilibrium is stable if this force overcomes gravity, i.e. if

$$\overline{mkv^2} > mg \sin \theta, \quad (1)$$

where the bar denotes the average over the period; the meaning of the remaining quantities is clear from Figure 4. To translate (1) into a useful criterion, we substitute $k = \theta / L + o(\theta)$, $v = u + o(\theta^2)$, and obtain,² for small θ :

$$\overline{u^2} > Lg, \quad (2)$$

the linearized stability criterion (see [3] for more details). Although this non-rigorous calculation looks suspiciously easy, it does give exactly the same result as the formal derivation due to Kapitza, as reproduced in Landau and Lifshitz [2] and almost a page long. Incidentally, (2) turns out to be equivalent to the stability condition $|\det F| < 2$ of the Floquet matrix F , providing a physical interpretation of this condition in terms of the centrifugal force of a non-existent constraint. To conclude, and as a side remark, a purely topological explanation of stability of the inverted pendulum, in a different regime, can be found in [4].

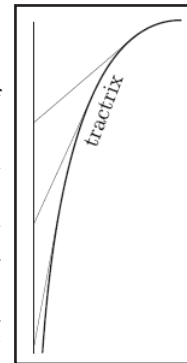


Figure 3. The tractrix, or the pursuit curve: all tangent segments have the same length.

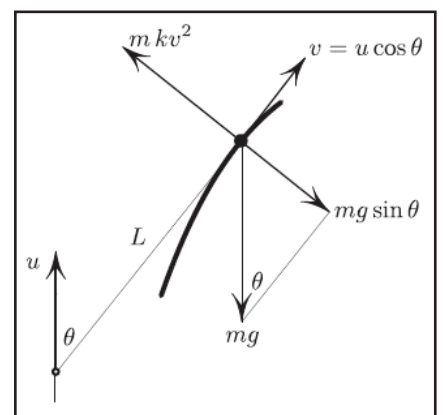


Figure 4. The centrifugal force mkv^2 of the non-existent constraint is responsible for stability.

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RandNLA

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been used in genetics, astronomy, climate science, and mass spectrometry imaging.

RandNLA algorithms have also led to the best worst-case bounds for problems such as least-squares approximations and variants of the low-rank matrix approximation problem. In recent years they have begun to penetrate numerical linear algebra in many ways, leading to new research and software such as Blendenpik and IBM's Skylark.

RandNLA has grown rapidly over the last 15 years. The 4th edition of Golub and van Loan's Matrix Computations contains a special section on randomized low rank approximations and the CUR, a strong indication that RandNLA is now reaching the mainstream. The massive scale of today's problems in applications ranging from scientific simulations to data analytics requires the development of novel, disruptive methods, and randomization via RandNLA has proven effective in the design and analysis of matrix algorithms. The area has achieved a level of maturity allowing basic methods to be taught to a broad range of graduate students; thus, the timing for G2S3 2015 was ideal.

G2S3 activities took place at the European Cultural Centre of Delphi (ECCD), which also housed participants. Fittingly, the ECCD was built to bring people together in the spirit of the ancient Delphic tradition of cultural exchange.

The school was organized around talks on the following themes in RandNLA: sampling, numerical aspects, statistical and optimization aspects, random projections, and linear algebra and MATLAB tools. Many of the participants commented favorably on the opportunity to socialize and network with their peers and the instructors, an integral component of all G2S3s. Students participated in an open problems session and also presented their ongoing or planned research (sometimes outdoors, profiting from the art-filled yards and the breathtaking view of the valley at Delphi). Eugenia Kontopoulou demonstrated the RandNLA GUI for the TMG MATLAB toolbox built at the University of Patras.

In addition to the educational activities, participants also enjoyed a guided tour of ancient Delphi, visited the Delphi Museum and its Charioteer statue, and took a day-long bus ride along the Corinthian Bay to the Rio-Antirrio Bridge and the beautiful town of Lepanto.

Mathworks offered all participants access to the latest MATLAB tools. Admittedly, several participants were spotted using Python, ipython, and other frameworks more popular in machine learning and data analysis. This was despite the fact that according to one legend, Apollo had to slay a serpent dragon guarding the cult center (in order to found his own temple), which rotted as its blood dried up under the sun. In classical Greek, to rot is "pytho"

(ΠΥΘΩ), so the dragon became known as "python." The sunrays apparently turned the rotting dragon into Python!

Holding the RandNLA G2S3 at Delphi was a coincidence of sorts. Gene Golub was heavily involved in MMDS 2006², while several well-known contributors to RandNLA are Greek.

RandNLA techniques were recently used to negate a longstanding conjecture of the distinguished archeologist Sir Arthur Evans (who discovered the ancient palaces of the Minoans in Crete and defined the Linear A and Linear B scripts) regarding the ancestry of the early Cretans. According to a Homeric hymn, Apollo picked Delphi as a place "to make a glorious temple and an oracle for men." Delphi—the "navel of the world"—became a meeting point of pilgrims visiting from afar in search of oracular answers that would help cure their problems. Little did they know that some 2000 years later, Delphi would be the place where students of mathematics, computer science, and statistics would come to learn about the appropriate CUR for their data problems!

This year's G2S3 would not have been possible without SIAM. In spite of the maelstrom caused by the capital controls imposed on bank transactions in Greece the weekend following G2S3, the program was a success. Thanks are also due to the U.S. National Science Foundation for a significant grant supporting the travels of U.S.-based participants, ECCD staff for their hospitality and the University of Patras and its Computer Engineering and Informatics Department (CEID) for additional funding, efficient organization, and administration of finances.

To learn more:

Avron, H., Maymounkov, P., & Toledo, S. (2010). Blendenpik: Supercharging LAPACK's



Outdoor problem solving, with a view of the gardens. Eugenia Kontopoulou (Patras) at the blackboard.

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G2S3 participants posing at Delphi's Temple of Apollo.

² <http://mmds-data.org>