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Learning with Nonnegative Matrix Factorizations

By Nicolas Gillis

Identifying the underlying structures within large data sets is a crucial data science task, and numerous techniques exist to successfully do so. One of the oldest approaches is linear dimensionality reduction (LDR), which assumes that each data point is generated from a linear combination of a small number of basis elements. Given a data set of n vectors $x_i \in \mathbb{R}^p$ $(1 \leq i \leq n)$, LDR looks for a small number r of basis vectors $u_k \in \mathbb{R}^p$ $(1 \leq k \leq r \ll n)$, such that each data point is well approximated using a linear combination of these basis vectors; that is,

$$x_i \approx \sum_{k=1}^{r} u_k v_i(k) \quad \text{for all } i,$$

where the $v_i(k)$s are scalars. LDR is equivalent to low-rank matrix approximation (LRA) since one can equivalently write the previous equation as

$$\underbrace{[x_1, x_2, \ldots, x_n]}_{X \in \mathbb{R}^{p \times n}} \approx \underbrace{[u_1, u_2, \ldots, u_r]}_{U \in \mathbb{R}^{p \times r}} \underbrace{[v_1, v_2, \ldots, v_n]}_{V \in \mathbb{R}^{r \times n}},$$

where $v_i \in \mathbb{R}^r$ is the ith column of V and contains the weights to approximate x_i in the basis U; i.e., $x_i \approx Uv_i$ for all i. The rank-r matrix UV hence approximates the data matrix X.

When the solution (U,V) minimizes the sum of the squares of the residuals $X - UV$ (least squares), LRA recovers principal component analysis (PCA), which can be computed via the singular value decomposition. LRA is a workhorse in numerical linear algebra and relevant to a wide array of applied mathematics, including blind source separation in signal processing; regression, prediction, clustering, and noise filtering in statistics and data analysis; and system identification and model reduction in control and systems theory. Although PCA has existed for more than a century, LRA has gained much momentum in the last 20 years. The reason for this is mostly twofold: (i) data analysis has become increasingly important in recent years, particularly with the current big data era, and (ii) LRA—despite its simplicity—is very powerful since low-rank matrices can effectively approximate many high-dimensional data sets [3].

Researchers use LRA models as either compression tools or as direct means to identify hidden structures in data sets. Many variants of LRA have emerged over the past few years, with two key differences. First, the error measure can vary and should thus be chosen depending on the noise statistic assumed on the data. For example, PCA employs least squares, which implicitly assumes independent and identically distributed Gaussian noise. Using the ℓ_1 norm leads to robust PCA, which better tolerates outliers. Another significant variant occurs when data is missing, for which the error measure can only be based on the observed entries. Researchers have successfully utilized it for recommender systems that predict users' preferences for certain items. This was true of the Netflix Prize, a competition that sought the most efficient filtering algorithm to predict user film ratings based solely on previous ratings.

See **Matrix Factorizations** *on page 3*

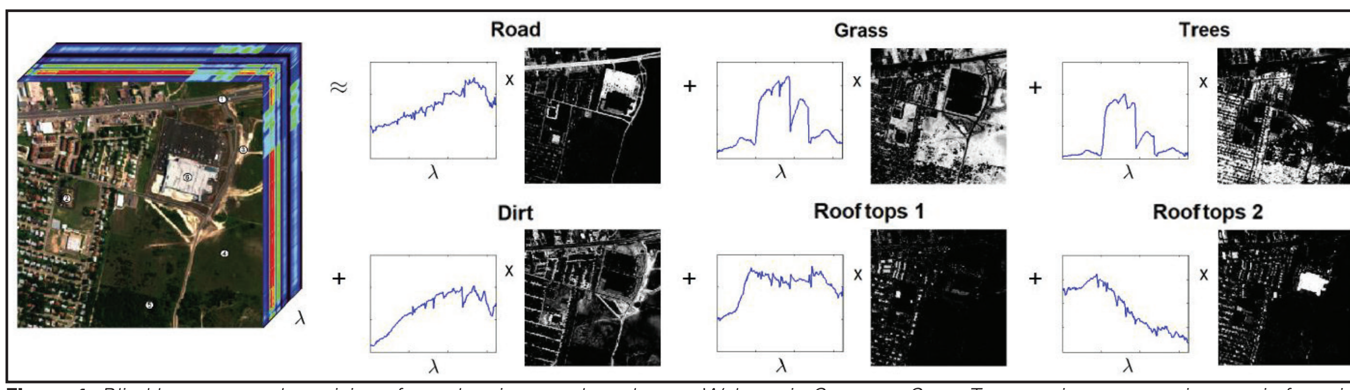

Figure 1. *Blind hyperspectral unmixing of an urban image taken above a Walmart in Copperas Cove, Texas, using nonnegative matrix factorization, with $r=6$ (162 spectral bands, 307×307 pixels). Each factor corresponds to the spectral signatures of an endmember (a column of U) with its abundance map (a row of V). Light tones represent high abundances. Image courtesy of Nicolas Gillis.*

Pentamode Materials: From Underwater Cloaking to Cushioned Sneakers

By Andrej Cherkaev, Muamer Kadic, Graeme W. Milton, and Martin Wegener

The fundamental fields of classic three-dimensional linear elasticity are the strain $\epsilon(\mathbf{x})$—the symmetrized gradient of the displacement field $\mathbf{u}(\mathbf{x})$, $\epsilon = [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]/2$—and the stress $\sigma(\mathbf{x})$. The stress $\sigma(\mathbf{x})$ is defined so that removing a small tetrahedron of material at $\mathbf{x}$ and loading this cavity's four faces by surface traction forces $\sigma \cdot \mathbf{n}_i$—where $\mathbf{n}_i$, $i=1,2,3,4$ are the normals to the cavity walls—means that the surrounding displacement field is essentially unchanged by the cavity's insertion. One can represent both $\epsilon(\mathbf{x})$ and $\sigma(\mathbf{x})$ in cartesian coordinates with symmetric 3×3 matrix-valued fields, also labeled $\epsilon(\mathbf{x})$ and $\sigma(\mathbf{x})$. In a homogeneous medium, these fields are linked by the constitutive law $\sigma(\mathbf{x}) = \mathbf{C}\epsilon(\mathbf{x})$, where $\mathbf{C}$ (the elasticity tensor) characterizes the material response and is a linear self-adjoint map on the space of symmetric 3×3 matrices. This space is six-dimensional. Thus, choosing a basis in the space of symmetric 3×3 matrices allows a symmetric 6×6 matrix to represent $\mathbf{C}$ and six-dimensional vector fields to represent $\sigma(\mathbf{x})$ and $\epsilon(\mathbf{x})$. Nonnegativity of the elastic energy $\epsilon(\mathbf{x}) \cdot \mathbf{C}\epsilon(\mathbf{x})/2$ then forces the matrix representing $\mathbf{C}$ to be positive semidefinite. Under special conditions, such as with prescribed displacements at a body's boundary, the elastic energy need only be quasiconvex rather than nonnegative.

Is this inclusive of all the constraints on $\mathbf{C}$, or might there be some hidden restrictions? We first addressed this question in 1995, ultimately demonstrating that given a positive definite symmetric matrix $\mathbf{C}$, one could find a microstructure built from two isotropic materials—one sufficiently stiff and the other sufficiently compliant—such that $\mathbf{C}$ is the matrix representing its effective elasticity tensor [8]. There are consequently no hidden restrictions on $\mathbf{C}$. The introduction of a new class of elastic materials called pentamode materials, for which $\mathbf{C}$ is essentially a rank-one tensor, was key to this result. The "null space" of $\mathbf{C}$ is five-dimensional, hence the name "pentamode." Five independent strains ϵ_j exist in $\mathbf{C}$'s null space and cost negligible elastic energy when applied to the material. We can write $\mathbf{C} \approx \mathbf{A} \otimes \mathbf{A}$, where the 3×3 matrix $\mathbf{A}$ represents the stress that the structure supports.

The simplest pentamodes are fluids with $\mathbf{A} = \sqrt{\kappa}\mathbf{I}$, where κ is the bulk modulus and gels—being close to fluids—display almost the same ideal behavior. Ole Sigmund used topology optimization to numerically identify other constructions with "fluid-like" effective elasticity tensors of this form [10]. Independently, we designed a complete family of pentamodes that allow for any matrix $\mathbf{A}$ [8]; like fluids, they only support one loading (up to a multiplicative constant). Unlike with fluids, this loading is not necessarily hydrostatic, but can be arbitrary and thus expressible as a combination of a hydrostatic and shear loading [5, 8].

Our pentamode design consists of double-cone elements arranged in a diamond-like structure (see Figure 1). The tips of precisely four double-cone elements meet at any vertex in the structure. By balance of forces, the tension in one double-cone element thus uniquely determines the tension in the other three that meet it — and by induction, the tension in every double-cone element in the structure. The mate-

See **Pentamode Materials** *on page 4*

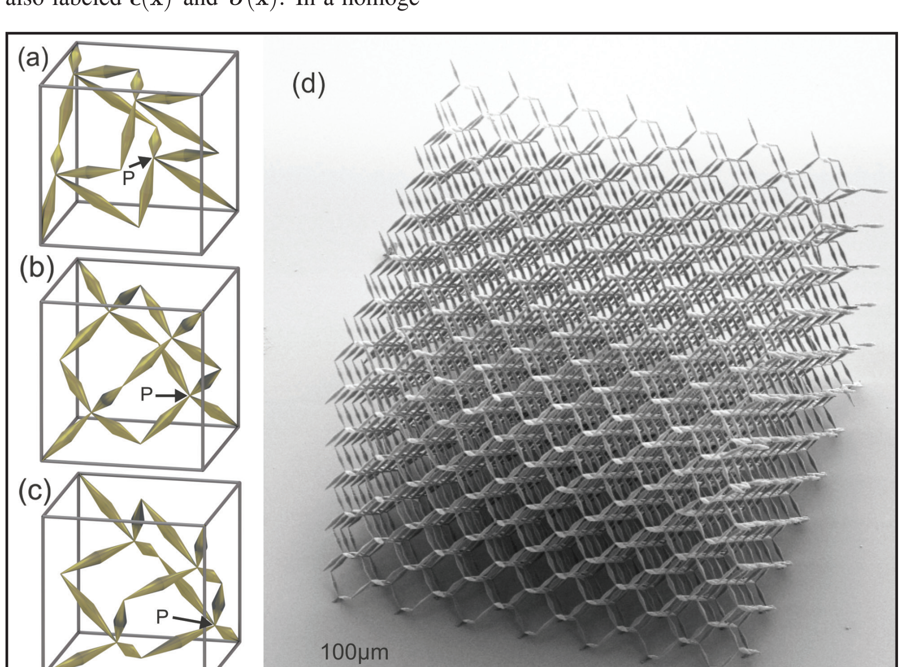

Figure 1. *Visualization of pentamodes.* **1a-1c.** *These computer-generated images each show four primitive unit cells of pentamodes in varying degrees of anisotropy, as dictated by the position of point P in the unit cell. 1b corresponds to the pentamode that supports a loading $\mathbf{A}$ proportional to $\mathbf{I}$.* **1d.** *An electron micrograph of a pentamode corresponding to 1b, built with three-dimensional laser lithography. Image courtesy of Tiemo Bückmann.*

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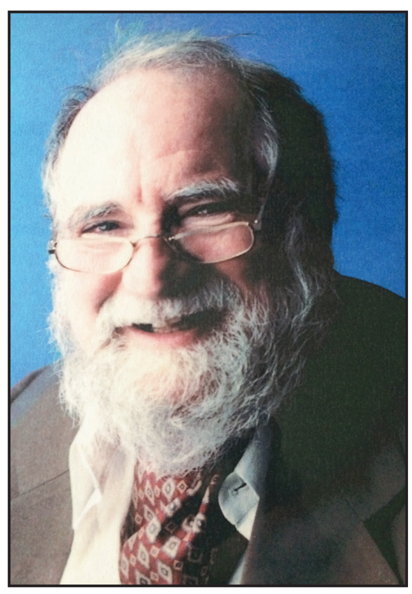
Obituary: Andrew R. Conn

By Michael L. Overton

Andrew R. Conn, known to everyone as Andy, was born in London on August 6, 1946, and passed away in Westchester County, NY, on March 14, 2019. He played a pioneering role in nonlinear optimization and remained very active in the field until shortly before his death.

Andy obtained his B.Sc. with honors in mathematics at Imperial College London in 1967 and then moved to Canada, earning a master's degree in computer science from the University of Manitoba in 1968. Opting to study in one of the world's coldest places turned out to be an extraordinarily happy choice for Andy because he met Barbara, his wife of nearly 50 years, in Winnipeg. Andy continued his studies at the University of Waterloo and received his Ph.D. from the Department of Applied Analysis and Computer Science in 1971. He completed a year-long postdoctoral fellowship at the Hebrew University of Jerusalem before returning to Waterloo in 1972 as a faculty member, first in the department that awarded his Ph.D. (later renamed the Department of Computer Science), and then in the Department of Combinatorics and Optimization. In 1990, after 18 years at Waterloo, Andy moved to IBM's Thomas J. Watson Research Center in Yorktown Heights, NY. The two halves of his research career at these respective institutions were completely different; he detailed his career trajectory in a fascinating article entitled *My Experiences as an Industrial Research Mathematician*, which appeared in a previous issue of *SIAM News* [4].



Andrew R. Conn, 1946-2019. Photo courtesy of Barbara Conn.

Andy's research interests were extensive but centered on nonlinear optimization. His work was typically motivated by algorithms and included convergence analysis, applications, and software. According to Google Scholar, Andy had more than 100 publications with at least 10 citations — and over 14,400 citations in total. His first published paper, "Constrained Optimization Using a Nondifferentiable Penalty Function" [3], appeared in the *SIAM Journal on Numerical Analysis* in 1973 and was quite influential in paving the way for the widespread use of exact penalty functions in nonlinear programming. Andy's work with Richard H. Bartels and James W. Sinclair on linear l_1 approximation [1] was another important early-career paper. He had 10 Ph.D. students at the University of Waterloo, including Paul Calamai, Thomas F. Coleman, and Yuying Li — all of whom are currently professors there.

In the late 1980s and 1990s, Andy maintained an extraordinarily productive collaboration with Nicholas I.M. Gould and Philippe L. Toint that resulted in more than 20 publications by these three authors alone. *Trust Region Methods* [6], the first book in the *Mathematical Optimization Society (MOS)-SIAM Series on Optimization*, was a highlight of this partnership. Other noteworthy contributions include the LANCELOT software for large-scale constrained optimization [5]—for which Andy, Gould, and Toint received the 1994 Beale – Orchard-Hays Prize for Excellence in Computational Mathematical Programming—and the influential Constrained and Unconstrained Testing Environment (CUTE) [2].

In recent years, Andy became interested in derivative-free optimization (DFO). Together with Katya Scheinberg and Luis Nunes Vicente, he published several papers on this topic and a book titled *Introduction to Derivative-Free Optimization* [7], for which the trio was awarded the 2015 MOS-SIAM Lagrange Prize in Continuous Optimization. The citation states that the book "includes a groundbreaking trust region framework for convergence that has made DFO both principled and practical."

Although Andy's research was predominantly devoted to continuous nonlinear optimization, he had an ongoing interest in applications involving mixed integer nonlinear programming and differential equations. He collaborated with several colleagues at IBM to apply nonlinear optimization to circuit-tuning problems, ultimately developing a system that has significantly impacted IBM's circuit design. Along with Ruud Haring and Chandu Visweswariah, he won an IBM Outstanding Technical Achievement Award for this work.

Andy was also no stranger to SIAM. He served as chair of the SIAM Activity Group on Optimization from 1992 to 1994, and was named a SIAM Fellow in 2013.

Andy was an extraordinary person, admired and respected by all who knew him. He had a passion for fairness, honesty, and openness, to the extent that he signed all of his referee reports — even the most negative. He loved sharing his knowledge through collaboration, teaching, and conversation; was continually supportive of friends and colleagues; and had a wonderful sense of humor. Lior Horesh, Andy's manager at IBM, spoke highly of him. "Beyond his remarkable scholastic accomplishments, Andy was a dear friend with great empathy and sense of humor, and a charming personality," Horesh said. "He was an incredible colleague with extraordinary insights, curiosity, and eagerness to solve complex problems." Many more tributes to Andy are available on the blog set up by his family.[1]

Andy was diagnosed with melanoma in 2013. Despite his serious illness and aggressive treatments, he remained very brave and amazingly cheerful during the last five years of his life. Andy celebrated his 70th birthday in 2016 with many colleagues at the Workshop on Nonlinear Optimization Algorithms and Industrial Applications,[2] which was held in his honor at the Fields Institute for Research in Mathematical Sciences. Naturally, he attended every talk and viewed most of the posters.

Just last summer, Andy attended the 23rd International Symposium on Mathematical Programming in Bordeaux, France, racing from session to session in his usual fashion and enjoying fine food and wine with friends and colleagues in the evenings. Three months before he died, he gave a wonderful talk at New York University entitled "An l_1-Augmented Lagrangian algorithm and why, at least sometimes, it is a very good idea"[3] — a perfectly Andy-esque title that conveyed content, enthusiasm, and a caveat all at once. Less than two weeks before his passing, he was explaining a math problem to one of his grandchildren with equally energetic enthusiasm.

Andy is survived by his wife Barbara, his mother and four siblings, his daughter Leah, his son Jeremy, and three grandchildren. He will be greatly missed by his family, friends, and the optimization community.

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Michael L. Overton is a professor of computer science and mathematics at New York University. He first met Andy Conn in 1979.

[1] https://arconn.home.blog/

[2] http://www.fields.utoronto.ca/activities/15-16/algorithms

[3] https://cs.nyu.edu/overton/AndyConnTalkNYU.pdf

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New Jersey High Schoolers Earn Top Honors for Mathematical Model of Substance Abuse

MathWorks Math Modeling Challenge Explores Drug Use among U.S. Population

By Lina Sorg

The use and subsequent abuse of substances like tobacco, alcohol, and narcotics are on the rise among teenagers in the United States. Electronic cigarettes and vaping—inhalation of an aerosol produced by vaporization of liquid chemicals like nicotine, a highly-addictive substance derived from tobacco—are popular with high school students, so much so that the U.S. Surgeon General declared e-cigarette use an epidemic among America's youth in late 2018.[1] Opioid addiction is also remarkably prevalent in the U.S., with increasingly more individuals abusing both prescription and non-prescription drugs. A 2019 report from the National Safety Council[2] indicates that Americans are now more likely to die of accidental opioid overdose than in a motor vehicle accident.

Substance abuse affects the physical and mental health of users and can interfere with brain development in adolescents. The numerous, wide-ranging consequences of addictive behavior extend well beyond individual users to society as a whole. Besides the evident health-related repercussions, such behavior negatively impacts finances, school and workplace performance, and social and familial relationships. Regulatory efforts at the local, state, and national levels attempt to control and restrict access to and consumption of addictive substances. In order to truly find success, such efforts must be rooted in a deep understanding of the ways in which substance abuse spreads among vulnerable populations.

The complicated dynamics of substance abuse made it a particularly relevant topic for this year's MathWorks Math Modeling (M3) Challenge,[3] a high school mathematics contest sponsored by MathWorks and organized by SIAM. The competition, which awards a total of $100,500 in scholarship funds, invites U.S. teams of high school juniors and seniors to tackle a multifaceted, real-world problem with mathematical modeling and report their results in only 14 hours. After two rigorous rounds of online and in-person judging by nearly 150 professional applied mathematicians, the top six teams traveled to New York City to present their solution papers in front of one last panel of judges and compete for the grand prize of $20,000. This final event was hosted in late April by Jane Street, a New York-based quantitative trading firm.

The three-part Challenge problem[4] asked students to create a mathematical model that predicts the spread of vaping in coming years; calculate the likelihood that certain individuals among a class of 300 high school seniors will use nicotine, marijuana, alcohol, and unprescribed opioids; and analyze the broader impacts of substance abuse. "This is a problem that can be approached from a variety of different ways, depending on the students' comfort zone with mathematics but also because of their own experiences," said judge Kathleen Kavanagh (Clarkson University), who co-wrote the 2019 problem with Karen Bliss (Virginia Military Institute) and Ben Galluzzo (Clarkson University). "I really feel like each student is going to have some sort of exposure to issues that are centered on addiction, and they can bring that into their solution. I think it's something to which they can automatically relate."

This year's first-place team, from High Technology High School in Lincroft, NJ, likened the spread of conventional cigarette and e-cigarette use to that of an infectious disease during an epidemic. "In order to use a drug you have to know someone who uses it, or have watched someone online who's used it, like in advertisements," Eric Chai of High Technology said. "That's kind of similar to how infections must be contracted from a person." Chai and his teammates thus derived their initial model from a SIRS (susceptible-infected-recovered-susceptible) compartmental model and adapted it to acknowledge that a relapsing individual would re-enter the "infected" rather than "susceptible" category. Using their model, they solved a system of differential equations to analyze both cigarette and e-cigarette use in the coming decade. The students concluded that 26.63 percent of Americans will vape in 2029, while only 6.45 percent will smoke cigarettes.

See **Substance Abuse** *on page 4*

[1] https://e-cigarettes.surgeongeneral.gov/documents/surgeon-generals-advisory-on-e-cigarette-use-among-youth-2018.pdf

[2] https://injuryfacts.nsc.org/all-injuries/preventable-death-overview/odds-of-dying/

[3] https://m3challenge.siam.org/

[4] https://m3challenge.siam.org/archives/2019/problem

Matrix Factorizations

Continued from page 1

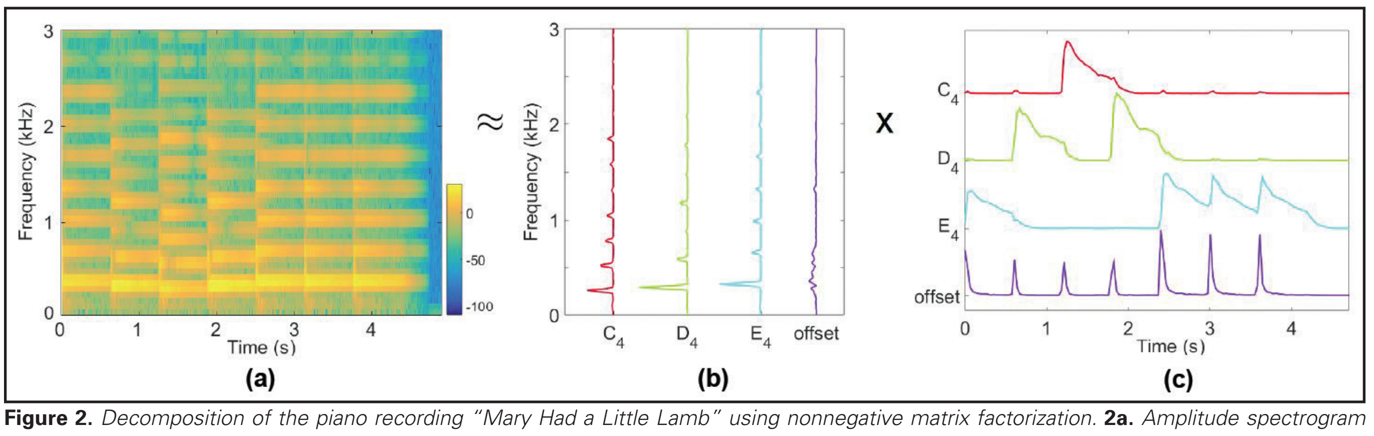


Figure 2. *Decomposition of the piano recording "Mary Had a Little Lamb" using nonnegative matrix factorization.* **2a.** *Amplitude spectrogram X in decibels.* **2b.** *Basis matrix U corresponding to the notes C_4, D_4, and E_4.* **2c.** *An offset activation matrix V that indicates when each note is active. Image courtesy of Nicolas Gillis.*

Second, one can impose varied constraints on the factors U and V to achieve different goals. In PCA, the factors are orthogonal and ordered in terms of importance. If a user instead wants to explain each data point with the minimum number of basis vectors, every column of matrix V should contain as many zero entries as possible. This LRA variant is called sparse component analysis and is closely related to dictionary learning and sparse PCA.

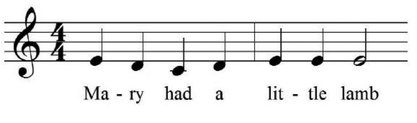
Among LRA models, nonnegative matrix factorization (NMF) requires factor matrices U and V to be component-wise nonnegative. Pentti Paatero and Unto Tapper first introduced NMF in 1994; it then gained momentum with the seminal paper of Daniel Lee and Sebastian Seung in 1999 [2]. Because of the additional nonnegativity constraints, NMF has a higher fitting error than PCA. Therefore, one should employ it when the factors U and V allow for the identification of hidden structures in a data set, e.g., when their entries are physical quantities.

Blind Hyperspectral Unmixing

A hyperspectral image (HSI) records the spectral signature of each pixel by measuring the reflectance (fraction of reflected, nonnegative light energy) for up to 200 different wavelengths. Physical materials reflect different amounts of light at different wavelengths, and are hence identifiable by their spectral signatures. Blind hyperspectral unmixing (blind HU) aims to recover the materials present in an HSI—called the endmembers—along with the abundances of every endmember in each pixel (which are also nonnegative) without prior knowledge of the materials or their properties. The linear mixing model (LMM) is the most standard model for blind HU. It assumes that each pixel's spectral signature is a linear combination of the endmembers' spectral signatures, where the weights are the abundances of the endmembers in that pixel. For example, if a pixel contains 50 percent grass and 50 percent road surface, its spectral signature will be equal to half of the spectral signature of grass plus half of the spectral signature of the road surface. This is because half of the light hitting that pixel is reflected by the grass and the other half is reflected by the road. When constructing matrix X so that each column is a pixel's spectral signature, the LMM translates into NMF — where the columns of U contain the endmembers' spectral signatures and the columns of V contain the abundances of these endmembers in each pixel. Figure 1 (on page 1) illustrates this decomposition.

Audio Source Separation

Given an audio signal recorded from a single microphone, one can construct a magnitude spectrogram. The signal is split into small time frames with some overlap (usually 50 percent). A user applies the short-time Fourier transform on each time frame and obtains the corresponding column of X by taking the magnitude of the Fourier coefficients. A piano recording of "Mary Had a Little Lamb," whose musical score is shown below, is a very simple monophonic signal for illustrative purposes.



The sequence is composed of three notes: C_4, D_4, and E_4. Figure 2 depicts the NMF decomposition of the magnitude spectrogram using $r=4$. The three notes are extracted as the first three columns of U (the signature of each note in the frequency domain), and a fourth "note" (last column of U) captures the first offset of each note in the musical sequence (common mechanical vibration acting in the piano just before triggering a note). The rows of V provide the activation of each note in the time domain. NMF is consequently able to blindly separate the different sources and identify which source is active at a given moment in time. Note that NMF reaches its full potential in polyphonic music analysis, when several notes and even several instruments are played simultaneously.

Other applications of NMF include extracting parts of faces from sets of facial images, identifying topics in a collection of documents, learning hidden Markov models, detecting communities in large networks, analysing medical images, and decomposing DNA microarrays [1]. In these instances, NMF's power stems from the interpretability of factors U and V. It would not be possible to interpret the PCA factors for the two aforementioned applications as done with NMF (e.g., as physical quantities that can only take nonnegative values). Due to the nonnegativity constraints, NMF's U and V factors automatically have some degree of sparsity.

Key considerations of NMF usage inspire important research questions for both NMF and other LRA models. A first critical question is as follows: *How does one ensure that the recovered factors correspond to the true factors that generated the data?* For instance, how can one be certain that matrix U will correspond to the true endmembers in blind HU or the true sources in audio source separation? In fact, NMF decompositions are in general not unique and thus require additional assumptions (such as sparsity of U and/or V) to guarantee that the computed decomposition matches that which generated the data [1]. A second vital issue concerns the *practical computation of NMFs*. NMF is NP-hard. In practice, most NMF algorithms are heuristics based on alternatively updating U and V. Yet in some cases, one can provably solve NMF in an efficient manner. For example, this is possible in blind HU in the presence of pixels containing only a single endmember. Other areas of ongoing research include model-order selection (choice of r) and choice of the objective function.

Despite the surge in interest over the past 20 years, the intricacies of solutions to this straightforward but subtly difficult problem mean that an abundance of elegant theoretical opportunities are still available for NMF. Given the breadth and practicality of its applications, NMF is clearly gaining momentum as a fundamental tool for understanding latent structure in data.

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Nicolas Gillis is an associate professor in the Department of Mathematics and Operational Research at the University of Mons in Belgium. His research interests include numerical linear algebra, optimization, signal processing, machine learning, and data mining.

Substance Abuse

Continued from page 3

When simulating the likelihood that a given individual will use nicotine, marijuana, alcohol, or unprescribed opioids, the New Jersey team utilized a binary multivariate logistic model to ensure inclusion of a variety of influencing factors and social attributes collected from the 2005-2006 Health Behavior in School-Aged Children survey.[5] Their model assessed the effects of the following factors on substance abuse: age, gender, ethnicity, income, overall health, relationships with friends and parents, opinions on school, weapon possession, and experience with bullying. "We basically trained the logistic equation so that given new data, we could predict the output of probability that someone would use a substance," team member Gustav Hansen said. The team then coded and employed a Monte Carlo simulation that generated 300 high school seniors with varying attributes. They found that 46.3 percent of those students would use nicotine, 17.3 would use marijuana, 66.0 percent would use alcohol, and 0.0 percent would use opiates.

Finally, the High Technology team developed a robust metric to rank the impact of the four aforementioned substances. They split the effects of these drugs into four categories: physical harm, social harm, dependence, and economic harm. The students measured the first three factors on a scale of 0 to 3 based on psychiatric survey results, and defined economic harm as the loss of gross domestic product from the decrease in life expectancy caused by substance abuse. "We also provided harm values on an individual and societal level," Chai said. "Since certain drugs have a much lower population of use, we thought it would make sense to give both numbers, depending on how harmful the drugs are to one person or to the U.S. as a whole." On an individual level, the ranking from most to least harmful was opioids, alcohol, cigarettes, and marijuana. But in terms of societal impact, the ranking switched to alcohol, cigarettes, marijuana, and opioids. In this case, alcohol was the most harmful despite the often-fatal effects of opioids because the latter has a much smaller population of users.

Chai and Hansen—along with teammates Emily Jiang, Kyle Lui, and Jason Yan—will split $20,000 in scholarship funds for their first-place finish. The group also received the third-place M3 Challenge Technical Computing Scholarship Award, which yields an additional $1,000. Instituted in 2018 under the MathWorks title sponsorship, this prize is awarded for "outstanding use of programming to analyze, design, and conceive a solution for the problem" and allocates a total of $6,000 to three high-performing teams.

Seniors Chai and Lui are no strangers to the M3 Challenge; they also competed in last year's competition as juniors and made it to the final round. As they prepare for college, Chai reflected on his potential career trajectory. "Before participating in this challenge, I was always interested in math and computer science," he said. "But now I'm less interested in the purely theoretical stuff and more into data science, big data, analyzing trends and marketing, and things like that. I like how it has a real-world impact, and you can see the actual application in what you're doing."

In addition to presenting their solution papers in New York, all six finalist teams had the opportunity to hear from and converse with M3 Challenge alumnus Chris Musco, a current research instructor of computer science at Princeton University who will soon join the faculty of New York University's Tandon School of Engineering. Musco was a member of the 2008 finalist team from the Wheeler School in Providence, RI. Following his team's success, he studied applied mathematics and computer science at Yale University before earning his Ph.D. in computer science from the Massachusetts Institute of Technology.

Musco also served as a judge during the triage round of judging, reviewed an early draft of the problem statement, and was eager to encourage students and give back to the competition that first piqued his interest in applied mathematics. "I learned through the M3 Challenge that it's actually possible to not just use math as a tool, but to spend a career building new mathematical tools to apply in all sorts of different fields," he said. "This competition was a jumping-off point for me. At the time it really opened my mind to the fact that there's a potential for careers where I can keep doing math, possibly for the rest of my life."

High Technology High School's winning paper is available online.[6]

Lina Sorg is the associate editor of SIAM News.

[5] https://www.icpsr.umich.edu/icpsrweb/NAHDAP/studies/28241

[6] https://m3challenge.siam.org/sites/default/files/uploads/Team_12038_FINAL_0.pdf

The MathWorks Math Modeling Challenge 2019 championship team from High Technology High School in Lincroft, NJ, will split $20,000 in scholarship funds for their first-place model of substance abuse. From left to right: Eric Chai, Gustav Hansen, Emily Jiang, Jason Yan, and Kyle Lui. SIAM photo.

Pentamode Materials

Continued from page 1

rial's stress is hence uniquely determined (up to a multiplicative constant). Moving the vertex **P** where four double-cone elements meet within the unit cell—and applying an affine transformation to the structure if needed—lets one obtain any desired matrix **A**. Even pentamodes with **A** proportional to **I** are interesting, as they can be more "rubbery than rubber" in the sense that they may have a greater ratio of bulk to shear modulus. When we began this work in 1995, we never dreamed that pentamodes would actually be built. 17 years later, in collaboration with Tiemo Bückmann, Nicolas Stenger, and Michael Thiel, we managed to construct them via three-dimensional laser lithography techniques [6] (see Figure 1d, on page 1). Now they attract considerable attention (see, for example, the references in [7]).

Pentamodes are the building blocks for obtaining any elasticity tensor; for this reason, we call them the grandfather of all linearly elastic materials [2]. Roughly speaking, one may superimpose six pentamode structures—deforming them to avoid collisions if necessary—each of which supports a stress $\mathbf{A}_i$, $i = 1, 2, \ldots, 6$. Inserting a very compliant material (like foam) in the space between the six structures ensures that they all share the same average strain when the entire arrangement is deformed. As a result, the overall effective elasticity tensor is loosely the superposition of the elasticity tensors of the six pentamodes $\mathbf{C}_* \approx \Sigma_i \mathbf{A}_i \otimes \mathbf{A}_i$. This achieves our objective, since any symmetric positive definite 6×6 matrix can be represented in this form. In fact, one can go even further and theoretically obtain all possible nonlocal effective behaviors in linear elasticity [4].

Interest in pentamodes grew when the material was affiliated with underwater cloaking of acoustic waves [9]. Pentamodes can guide waves around an object if one chooses a suitable field $\mathbf{A}(\mathbf{x})$ and uses the appropriate pentamode at point $\mathbf{x}$. If $\mathbf{C} \approx \mathbf{A} \otimes \mathbf{A}$ matched the elasticity tensor of water (itself a pentamode) and shared water's overall density at the outer surface of the pentamode cloak, there would be no "impedance mismatch" to reflect the waves at this interface. Researchers have also proposed pentamode-inspired constructions between stiff horizontal plates for seismic insulation [1]. Such constructions would allow the plates to slide with respect to each other and with little change in their spacing. The ground underneath could move horizontally while the top plate (above which lies the protected structure) would remain relatively still.

One can also use pentamodes to construct an "unfeelability cloak" for static elasticity [3]. In Hans Christian Andersen's *The Princess and the Pea*, the "true princess" might have failed to feel the pea underneath her mattresses if the mattresses had an appropriate pentamode construction designed to shield the pea from compressive forces. Who knows, perhaps pentamode mattresses will be built; they would be much lighter than water beds. Interestingly, Adidas' "Futurecraft" sneakers have a lattice construction in their soles, which perhaps may make a stone less discernable.

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Andrej Cherkaev and Graeme W. Milton are mathematicians at the University of Utah. Muamer Kadic is a physicist at the FEMTO-ST Institute, associated with the French National Center for Scientific Research at the Université Bourgogne Franche-Comté in Besançon, France. Martin Wegener is a physicist at the Institute of Applied Physics and Institute of Nanotechnology at the Karlsruhe Institute of Technology in Germany.

SIAM Joins Societies Consortium on Sexual Harassment in STEMM

On February 15, 2019, leading academic and professional societies officially announced the launch of a new Societies Consortium on Sexual Harassment in STEMM (science, technology, engineering, mathematics, and medicine). The consortium is meant to encourage and support ethical and professional conduct across the aforementioned fields, and SIAM is among the 100 foundational member societies.

Like the other member organizations, SIAM believes that professional societies are standard-setters for STEMM fields and thus responsible for addressing and preventing gender or sexual harassment that occurs in these areas. All participating societies agree to help with the creation and deployment of influential resources pertaining to sexual harassment for both individuals and broader associations within STEMM. The consortium will also serve as a forum for diverse leadership in its support of ethics, inclusion, equity, and merit in STEMM-related education, research, and implementation.

The Societies Consortium was established by the American Association for the Advancement of Science, the Association of American Medical Colleges, and the American Geophysical Union, with law and policy consultation from the EducationCounsel. SIAM is proud to pledge its support in the address and ultimate eradication of gender and sexual harassment in STEMM fields.

Perspectives on Teaching Math Modeling in High School

By Greta Mills

Let's create a post-calculus course in mathematical modeling! I couldn't have known that this one decision would drive my teaching philosophy moving forward. In late 2000, after attending the weeklong National Computational Science Education Consortium, I approached my department chair at Hanover High School in New Hampshire about creating a class that would build on this "new" idea of mathematical modeling. At the time, Hanover students who had completed calculus would typically take upper-level math classes at Dartmouth College, which is within walking distance of the school. But this often presented scheduling conflicts, so a high school course on mathematical modeling seemed like the next logical step. Such a class would give students the opportunity to encounter messy, real-world problems that require the formulation and application of assumptions, then iterate their processes to refine results. In the spring of 2002, Hanover High School offered math modeling for the first time.

Why Teach Modeling?

Guidelines for Assessment and Instruction in Mathematical Modeling Education (*GAIMME*),[1] a report written by education advocates, university professors, and K-12 teachers, defines mathematical modeling as "a process that uses mathematics to represent, analyze, make predictions, or otherwise provide insight into real-world phenomena" [1]. When I first started teaching, students regularly asked me when they would use mathematical concepts in the "real world." I spent a lot of time trying to convince them of the many fields that employ algebra, geometry, or calculus. I racked my brain for applications that would speak to their interests and reflect the class material's practicality. While some students accepted my explanations at face value, many indicated that they were not planning to pursue any related fields. Additionally, most high school concepts bear little resemblance to their real-world applications, especially at the lower levels. Students could thus tell when I was "stretching" the connection between their classroom math and any future utilization.

Over time, I realized that the question "When are we going to use this?" was actually about students' frustration or anxiety with the difficulty of mathematical topics. It is easier for them to make peace with their math troubles if they convince themselves that math has no relevance to their daily lives. Modeling gives students that relevance by providing context to the mathematics in question and letting them make real, impactful decisions about a problem. They learn how to prioritize issues, make assumptions, and analyze their solutions. For example, my current modeling class has been investigating lunch lines because of frequent congestion in the cafeteria. We first studied queue theory—made tangible by the context of cafeteria lines—to understand line functionality. Students have also had to contend with real issues like budgets, scheduling, and building codes.

I recently attended the "Critical Issues in Math Education" workshop, which took place in Berkeley, Calif., this past March and was sponsored by the Mathematical Sciences Research Institute. The overarching theme pertained to the following question: *How can we individually and collectively advance the teaching and learning of mathematical modeling in K-16*? The panelists and presenters represented a diverse set of stakeholders, including university professors and industry leaders. Many universities now offer graduate degrees in mathematical modeling, and a quick internet search for jobs involving "math modeling" returns hundreds—if not thousands—of positions in data science, analytics, and more. Our biggest stakeholders in the future of math modeling are the students themselves, who risk being left behind in this next wave of technological and industrial advancement without a foundation in modeling techniques.

Introducing Modeling: First Steps

In my experience, one of the biggest obstacles in transitioning a conventional classroom into one that supports a modeling mindset is the resulting tension between a more traditional, textbook-dependent curriculum and the open-ended nature of modeling scenarios. This friction can create significant anxiety for teachers who genuinely want to get a taste of modeling but do not know where to begin. Introducing modeling problems also requires ceding some classroom control; students are not authentically invested in the problems if they do not possess a certain level of autonomy in the process.

For teachers who are not quite ready to dive into the deep end of modeling, breaking down the process and scaffolding the activities into "bite-sized" explorations can ease them into modeling while acclimating students to a more collaborative, inquiry-based form of mathematics instruction. The Math Modeling Hub[2] and the Math Modeling Faculty Mentoring Network[3] both provide online resources and support for instructors at the K-16, graduate, and industry levels. In addition to *GAIMME*, numerous resources offer guidance and motivation for teachers, including SIAM's *Math Modeling: Getting Started and Getting Solutions* and *Math Modeling: Computing and Communicating*.[4]

Opportunities also exist for students and teachers to grapple with a modeling problem without sacrificing content or class time. High school modeling contests have increased in number and scope after I introduced modeling to my curriculum in 2002. Since 2004, I have had teams participate in the High School Mathematical Contest in Modeling (HiMCM), sponsored by the Consortium for Mathematics and Its Applications. Several teams have placed at or near the top over the years.

In 2011, my students first partook in the MathWorks Math Modeling (M3) Challenge,[5] a competition (formerly known as Moody's Mega Math Challenge) that SIAM has organized since 2006. In the spring of 2012, I served as the first high school judge for the M3 Challenge. I was incredibly nervous at the prospect of judging alongside some of the leading experts in mathematical modeling, but the judging process actually calmed my nerves. I could see that my students' efforts were in line with what other teams produced, and have enjoyed serving as a judge every year since.

HiMCM and the M3 Challenge have grown exponentially in recent years, and both contests provide students of all levels with the chance to work through open-ended, important, and real-world problems.

See **Math Modeling** *on page 8*

[1] https://www.siam.org/Portals/0/Publications/Reports/GAIMME_2ED/GAIMME-2nd-ed-final-online-viewing-color.pdf

[2] https://qubeshub.org/community/groups/mmhub

[3] https://qubeshub.org/community/groups/mmfmn

[4] Both handbooks are freely available online at https://m3challenge.siam.org/resources/modeling-handbook

[5] See page 3 for an article about this year's M3 Challenge.

A Comprehensive Exploration of George Boole

The Life and Work of George Boole: A Prelude to the Digital Age. *By Desmond MacHale. Cork University Press, Cork, Ireland, November 2014. 360 pages, $25.00.*

New Light on George Boole. *By Desmond MacHale and Yvonne Cohen. Cork University Press, Cork, Ireland, October 2018. 492 pages, $29.00.*

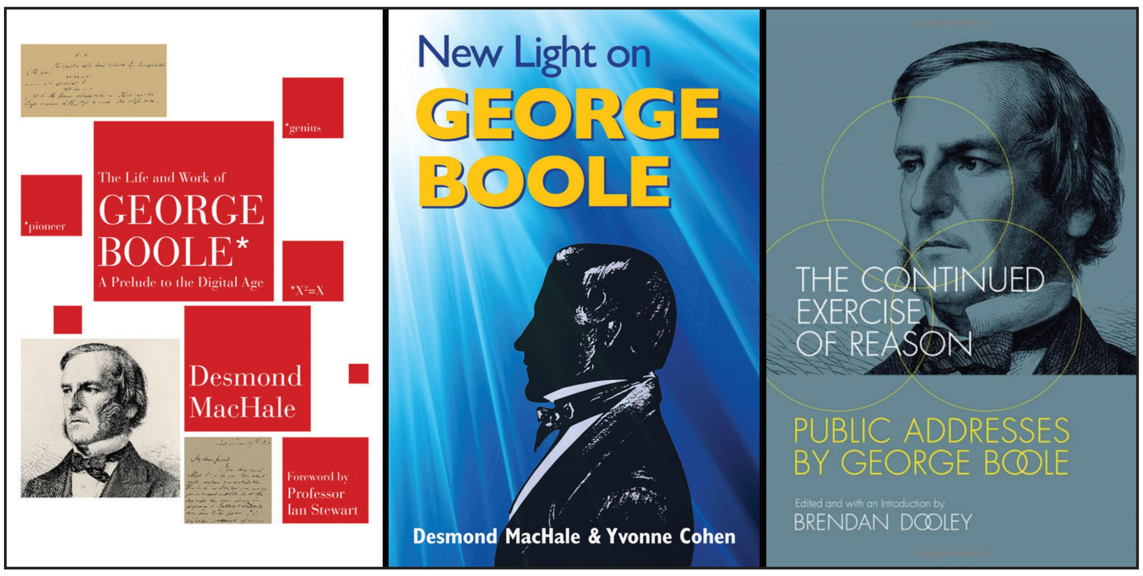
The Continued Exercise of Reason: Public Addresses by George Boole. *By Brendan Dooley (Ed.). The MIT Press, Cambridge, MA, April 2018. 248 pages, $34.00.*

BOOK REVIEW
By Ernest Davis

Boolean logic and Boolean algebra—the mathematics of *true* and *false*, of 1 and 0—are the foundation of essentially all digital computation and digital devices that pervade the modern world. George Boole himself (1815-1864) is less well known than his creations.

Yet Boole was an extraordinary figure in many ways, and his life deserves recognition. Fortunately, the labors of recent biographers have brought his name to the forefront of mathematical discussion. Mathematician Desmond MacHale published the first full-length biography of Boole, entitled *George Boole: His Life and Work*, in 1985. MacHale released a revised version in 2014 called *The Life and Work of George Boole: A Prelude to the Digital Age*. In 2018, he collaborated with Yvonne Cohen to publish additional material in *New Light on George Boole*. Historian Brendan Dooley also edited a collection, called *The Continued Exercise of Reason*, which contains all of Boole's surviving public lectures in addition to a 70-page introduction that provides historical and intellectual context.

Boole was born and raised in Lincoln, in the East Midlands of England. He was a conspicuously gifted child, though not especially so at math. At age 14, he published his own translations of three classical Greek poems in the local newspaper. In 1831, when Boole was 16 years old, he became a teacher to support his family after the collapse of his father's business. He advanced rapidly and opened his own school in 1834.



The Life and Work of George Boole: A Prelude to the Digital Age. By Desmond MacHale. New Light on George Boole. By Desmond MacHale and Yvonne Cohen. The Continued Exercise of Reason: Public Addresses by George Boole. By Brendan Dooley (Ed.). Images courtesy of Cork University Press and the MIT Press.

It was around this time that Boole began to seriously study mathematics. By his own account, he chose the subject because he had almost no money for books, and a math book would take longest to get through. Boole's mathematical education was entirely self-taught. He started with Sylvestre Lacroix's *Traité du Calcul Différentiel et du Calcul Intégral*, then worked through Isaac Newton's *Philosophiae Naturalis Principia Mathematica*, Joseph-Louis Lagrange's *Mécanique Analytique*, and Pierre-Simon Laplace's *Traité de Mécanique Céleste* (teaching himself French, German, and Italian along the way). Boole published his first paper, on the calculus of variations, in an 1838 edition of the *Cambridge Mathematics Journal*. In 1844, his paper titled "On a General Method for Analysis" won the Royal Society's first gold prize for mathematics. In 1849, Boole became a professor of mathematics at Queen's College in Cork, Ireland, where he taught for the rest of his life. He died at age 49 from pneumonia after walking through heavy rain to deliver a lecture.

Boole's fame rests predominately on his essential creation of mathematical logic in *The Mathematical Analysis of Logic* (1847) and *An Investigation of the Laws of Thought on Which are Founded the Mathematical Theories of Logic and Probabilities* (1854). But he made major contributions to other area of mathematics as well. In addition to Boolean logic, *The Laws of Thought* contains groundbreaking work on the foundations of probability theory. Boole was a major figure in the theory of differential equations and among the first people to formulate the concept of the differential operator. He wrote one of the earliest papers on invariants, thus laying the groundwork for Arthur Cayley's later development of the field. He also penned influential textbooks on differential equations and difference equations; the latter was not superseded until the 1930s.

Boole did have his gaps and blind spots. As far as I can tell, he made no contribution to geometry beyond teaching it every year. Despite his friendship with Cayley, he was uninterested in group and matrix theory. Most surprisingly, he apparently never realized that one must state the associative law as a separate axiom in Boolean algebra.

Religion was enormously important to Boole, and he struggled all his life to reconcile his rationalism with his Christian faith.

See **George Boole** *on page 7*

Which Energy is Greater?

In the opening scene of the movie *Men in Black*, a large dragonfly splatters across the windshield of an oncoming truck. As a result of the collision, the insect increases its near-zero pre-collision velocity to that of the truck and thus acquires kinetic energy. The contact also generates heat, as any inelastic collision does. Which of these two energies—kinetic or heat—is greater? The same question arises when a snowflake or rain droplet hits the windshield.

Interestingly, the two energies are equal (assuming that the dragonfly's pre-impact speed is negligible). To see why (and avoid calculation), let us examine the same event in two different frames of reference: first in the truck's and then in the ground observer's. In the truck's frame, the insect comes to a dead stop and slows from v (the truck's speed) to zero. All of its kinetic energy converts to heat,[1] so that acquired heat $H=mv^2/2$ (see Figure 1).

[1] Neglecting the small amount of energy that went into the sound, the windshield vibration, etc.

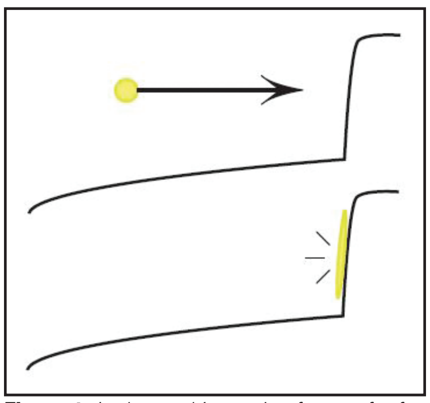


Figure 1. *In the truck's moving frame of reference, all the kinetic energy converts to heat.*

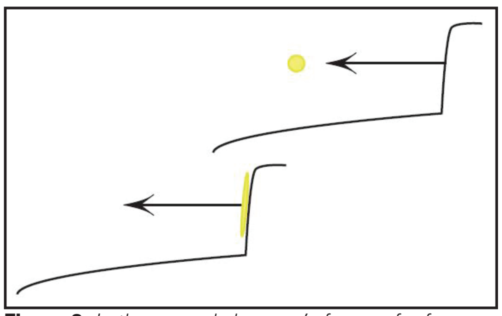


Figure 2. *In the ground observer's frame of reference, the acquired kinetic energy is* $\frac{mv^2}{2}$.

MATHEMATICAL CURIOSITIES
By Mark Levi

In the ground observer's frame, the dragonfly speeds up from zero to v, thus acquiring kinetic energy $K=mv^2/2$ so that $K=H$ as claimed (see Figure 2). The energy split is fair; half goes into the disordered heat motion and half into the ordered translational motion.

A Puzzle

Imagine that the truck instead hits a rubber ball of the same mass as the insect that (like the insect) has zero pre-collision speed. Assuming a perfectly elastic collision, the ball speeds up from zero to $2v$. Indeed, in the truck's frame the ball goes from $-v$ to v, which corresponds to acceleration from zero to $2v$ in the ground frame. The ball therefore acquires kinetic energy $\frac{m(2v)^2}{2}=4\frac{mv^2}{2}$. But this is more—exactly twice, in fact—than the total energy attained by the dragonfly! How can this be? Where did this extra $2\frac{mv^2}{2}$ come from?

The figures in this article were provided by the author.

Mark Levi (levi@math.psu.edu) is a professor of mathematics at the Pennsylvania State University.

Readers of *SIAM Review* React to *SIGEST* Section

SIAM surveyed readers of *SIAM Review* (*SIREV*) this January to gauge interest in and reactions to the *SIGEST* section, which highlights a recent paper (within the last four years) from one of SIAM's many specialized research journals. Survey results indicate that nearly two-thirds of respondents are in clear favor of the journal continuing to publish *SIGEST* papers.

SIGEST has been a fixture of *SIREV* for the past 20 years. The first-ever *SIGEST* selection—"Periodic Folding of Thin Sheets," by L. Mahadevan and Joseph B. Keller—appeared in a 1999 issue of *SIREV*.[1] Every subsequent issue of the quarterly publication has included a *SIGEST* paper. Selection of this article is notable, and authors are asked to revise their initial publication to appeal to a broader audience. Even before revision, the chosen papers are of interest to the entire SIAM community.

Nearly 1,000 *SIREV* readers replied to the survey and addressed the following points on a scale of "1" (strongly disagree) to "5" (strongly agree).

- I am aware of the *SIGEST* section of *SIAM Review* (weighted average of 3.44)
- I read the *SIGEST* section as frequently as I read other sections of *SIAM Review* (weighted average of 3.04)
- I have the impression that a typical *SIGEST* article reflects the aims and scope of the underlying SIAM journal (weighted average of 3.54)
- A typical *SIGEST* article is a good example of a high-quality, broad-appeal article from the underlying SIAM journal (weighted average of 3.69)
- SIAM provides a useful service by highlighting excellence through the mechanism of publishing *SIGEST* articles (weighted average of 3.81)
- *SIAM Review* should continue to publish a *SIGEST* article in each issue (weighted average of 3.88).

The breakdown of replies to the final question is as follows: 36.7 percent of respondents selected "5" (strongly agree), 29.1 percent selected "4," 23.6 percent selected "3," 6.5 percent selected "2," and 4.1 percent selected "1" (strongly disagree).

136 participants also offered a wide range of further comments. Some recommended increasing the number of *SIGEST* articles in each volume, while others suggested discontinuing *SIGEST* altogether. One respondent proposed highlighting "articles from different journals that address a theme or 'hot topic' in applied math to provide perspectives on that theme from different communities within SIAM."

SIREV editor-in-chief Des Higham (University of Edinburgh) reported to the *SIREV* Editorial Board that broad mandate exists for maintaining the status quo. He noted that a consistent theme in participants' comments was a desire for more widely-accessible *SIGEST* articles. Moving forward, Higham and the *SIREV* section editors will pay even closer attention to the selection of papers with broad appeal. Higham will also ensure that *SIGEST* authors—in making their revisions—maximize the opportunity to engage *SIREV*'s diverse readership of over 10,000 applied and industrial mathematicians.

[1] https://epubs.siam.org/doi/abs/10.1137/S0036144598339166

George Boole

Continued from page 6

In fact, a major underlying motivation for his study of logic was likely to determine the role of human reason in understanding God; *The Laws of Thought* includes a chapter on the logic pertaining to the theological arguments of Baruch Spinoza and Samuel Clarke. Additionally, Boole so much venerated theologian Frederick Denison Maurice that he had Maurice's photograph brought to him on his deathbed.

Beyond his teaching, Boole occasionally gave public lectures on a wide variety of subjects. Topics included a celebration of Newton, the origins of ancient mythologies, the social aspect of intellectual culture, the claims and philosophy of science, and the possibility of life on other planets (a prospect in which he believed). When a local social organization's library introduced a rule against acquiring books on controversial topics, Boole advocated to abolish the regulation. After the passage of a law that limited the work day to 10 hours, he delivered a talk entitled "The Right Use of Leisure" that encouraged people to read about science, history, and moral philosophy; partake in healthful exercise; and enjoy nature. Boole also spoke poignantly about education in a lecture that included insights from his personal experiences as a student and teacher. Some of these are pleasantly idiosyncratic; for instance, he emphasized the importance of good penmanship. Boole clearly had broad interests, was well-read, and possessed confidence in his ability to lecture on many topics.

His public addresses are not milestones in intellectual history by any means, but they do offer a window into the general mindset of Boole's time and place. Literary scholar George Herbert Palmer wrote that "the tendencies of an age appear more distinctly in its writers of inferior rank than in those of commanding genius." Boole was slightly younger than Charles Dickens, Charles Darwin, Abraham Lincoln, Benjamin Disraeli, Thomas Babington Macaulay, and Harriet Beecher Stowe, but seems much more "Victorian" in the somewhat pejorative stereotype. He embodied the turgid 19th-century lecture style—stiff, formal, long-winded, humorless, and often pompous—and possessed the smug certainty that 19th-century Christian Europe was the apex of human history. The incessant religiosity—in which any mention of the wonders or regularities of nature is followed by a pious reference to the "Author of Nature," and any mention of human activities is followed by a reference to man's "duty to his Creator"—is very characteristic of the era. Also characteristic is the sometimes-stifling level of propriety; in one lecture Boole warns against reading too many novels, and in another he worries about the corruptive dangers of exposing students to polytheist classical literature.

On the other hand, it is worth acknowledging that there is little in these speeches to offend a modern-day reader. It seems that Boole was rarely—if ever—sexist, racist, anti-Semitic, or anti-Catholic. He also does not defend slavery, imperialism, or the inferior status of women; you cannot count on that when reading most lectures from the 1840s.

One unexpected pleasure in Boole's biography is the figure of his wife, Mary Everest Boole. They married when he was 40 and she was 23, promptly had five daughters, and seemed to have had a happy marriage. Mary was an intelligent woman with a gift for math, and worked through Boole's entire textbook on differential equations while he was writing it. She was also something of a crackpot, particularly later in life; in fact, she may have inadvertently killed Boole by treating his final illness homeopathically and possibly insisting that he sleep in damp sheets.

Mary wrote a great deal, and in a much more lively and readable style than her husband. At her best she was strikingly insightful and even prescient. In 1868, she wrote that Charles Babbage and William Stanley Jevons "have conclusively proved, by unanswerable logic of facts, that calculation and reasoning, like weaving and ploughing, are work, not for human souls, but for clever combinations of iron and wood." At other times, she was charmingly nutty. "It is demonstrable that the faculties on which depend the possibility of logic and of algebra must have evolved in connection with an *intime* and private family life," she wrote. "Their source was — male and female engaged in peopling the world of the future."

Boole had no significant teachers and no significant students. He does not have a record in the Mathematics Genealogy Project, but his physical descendants were a remarkable bunch. His daughter Alicia conducted important work on four-dimensional geometry and discovered the six four-dimensional regular polytopes. Boole's daughter Lucy was the first woman professor of chemistry in England. His daughter Ethel Lilian Voynich wrote *The Gadfly*, a revolutionary novel that was immensely successful — particularly in the Soviet Union. And Boole's great-great-grandson Geoffrey Hinton is a leading figure in machine learning, continuing his ancestor's study of the mathematical analysis of *The Laws of Thought.*

Ernest Davis is a professor of computer science at New York University's Courant Institute of Mathematical Sciences.

Professional Opportunities and Announcements

Happy to be a Mathematician: Remarks to the AAAS Section on Mathematics

By David E. Keyes

David E. Keyes of King Abdullah University of Science and Technology (KAUST) was recognized as a 2018 Fellow of the American Association for the Advancement of Science (AAAS) Section on Mathematics for his service to the mathematical sciences profession and fundamental research contributions at the interface of parallel computing and numerical analysis. The following remarks are adapted and excerpted from his induction speech at the 2019 AAAS Annual Meeting, held in Washington, D.C., this past February.

As a mathematician, I consider myself to be one of most fortunate people in the world. In principle, anyone can access mathematics' beauty. But some of us were blessed to be encouraged to pursue the subject in our youth and are now able to make a living by doing mathematics as a profession. While we learned to love mathematics for its beauty, many of us also love it for its utility and community.

What is more beautiful than mathematics? One finds elegance in the pleasing structure of a proof, built brick-by-brick by lemmas or stepwise by induction. In a world where falsehoods are readily blended and sold with truth, mathematics offers access to an inner sanctum of truth and a paradigm for applying logical thinking to all of life's issues.

Beauty is also present in the magnificent structure of functions in the complex plane, so that an infinite real integral can be replaced with a set of infinitesimal contours around the poles of its integrand and evaluated based on a single term from an expansion at each pole. Equally breathtaking is the way in which an infinite polynomial—like the series for sine—converges everywhere on the real line to a number bounded in magnitude by one, something you would never guess if you camped on a large argument and watched the swinging term-by-term partial sums at the start.

Beauty is the readily visible or touchable riot of a Möbius strip or Klein bottle — one-sided surfaces embedded in higher dimensions. Another ultimate recreation for the mind is a space-filling curve, introduced as a mathematical curiosity by Giuseppe Peano in 1890 and David Hilbert in 1891. These one-dimensional curves get arbitrarily close to every point in a higher-dimensional space while recursively folding onto themselves so that the adjacent points in high-dimensional space are also near each other in arc length along the curve. Hilbert could never have guessed that over a century later, researchers would use these curves to lay out high-dimensional data in linearly-indexed computer memory to obtain proximity that is relevant to cache-based, distributed-memory computer architectures.

Speaking of computing, what about the mathematics of numerical analysis? We can now perform a quintillion—10^{18}—floating point operations per second in simulations that run for a week. After committing 10^{24} rounding errors with respect to exact arithmetic (following the compromise that is floating point), we can confidently bound the error in the result to a tiny fraction of unity. But computers at that scale burn barrels of oil per hour, so let's celebrate the beauty of algorithms that shave off full powers of the arithmetic complexity, which is the number of operations required to complete a computation.

The following are seven spectacular results of numerical analysis in improving computational complexity within my lifetime, occurring about once every decade:

- 1965: fast Fourier transform
- 1972: multigrid method
- 1986: fast multipole method
- 1991: sparse grids
- 1999: hierarchical matrices
- 2008: multilevel Monte Carlo methods
- 2011: randomized singular value decomposition.

What will be the next dramatic reduction in algorithmic complexity to reduce a polynomial-time task in the problem size to something linear or log-linear? I suspect that it will soon arise in the realm of deep learning. Stay tuned!

Let's go back to hierarchical matrices, which were introduced 20 years ago by Wolfgang Hackbusch and contemporaneously by Eugene Tyrtyshnikov. *H*-matrices approximate a dense matrix of size N^2 as a collection of blocks, almost all of which are representable through their singular value decomposition (or other cheaper means) to high accuracy with small rank. The result is a reduction of storage to $O(rN\log N)$, where r is the effective rank of a typical small block of the original matrix, and a reduction in the cost of multiplication, inversion, and other traditional matrix operations to $O(r^2 N\log^2 N)$.

Matrices with enough data sparsity to be compressed in this way are ubiquitous in practice. Hierarchical matrices are revolutionizing scientific computing and fitting unprecedentedly large problems into computer memory, which can never grow fast enough in our data-rich world.

This relates to my own research. My group is systematically introducing data sparsity into traditional linear algebra libraries and applications that rely on high-performance linear algebra. Examples of such applications include maximum likelihood estimation in the geospatial statistical prediction of weather or climate—like wind or solar insolation—to guide the placement of billions of dollars of renewable energy infrastructure.

In addition, Hessians for seismic inversion allow us to discover more oil until this renewable infrastructure is in place. Real-time adaptive optics help align mirrors of the largest land-based telescopes to correct for atmospheric turbulence. And density functional theory can design new materials. We work on these applications directly with scientists and engineers.

We also release open-source software—which has been picked up in the NVIDIA cuBLAS Library for millions of graphics processing units and the Cray Scientific and Math Libraries for hundreds of the top supercomputers—to reach a wider crowd.

The following four algorithmic premiums are important when migrating the world's scientific software to exascale computing:

• Massive load-balanced concurrency with minimal communication between distributed memory nodes

• Massive concurrency *within* the nodes for shared-memory cores

• High arithmetic intensity, namely restriction to data that already exists in registers and caches, due to the thousand-cycle penalties of going to DRAM or off-chip

• Synchronization reduction; as we head towards *one billion* one-gigahertz cores to achieve 10^{18} operations per second, synchronizing through traditionally addictive algorithmic idioms can pace the entire computation by the slowest or most data-starved core.

Ph.D. students in my current group must aim to improve at least one of these four aspects of an algorithm that manipulates a matrix, traverses a mesh, operates on an unstructured particle swarm, or extends existing exascale algorithms to a new application. Seven of the inaugural 10 graduates' first postdoctoral placements were funded by the U.S. Department of Energy.

So, how did I get here? I earned my bachelor's degree in mechanical engineering and engineering physics, and wanted to work on problems related to energy resources and conversion in the oil-embargoed 1970s. I discovered that mathematical modeling was my favorite part of engineering, so I pursued a Ph.D. in applied mathematics. The first commercial parallel computers emerged around this time, which inspired my postdoctoral research in computer science. My first faculty appointment was in mechanical engineering, during which I taught graduate-level applied mathematics while beginning my research in parallel computational fluid dynamics; this has remained my main interest.

The 2018 American Association for the Advancement of Science (AAAS) Fellows for the Section on Mathematics were recognized earlier this year at the 2019 AAAS Annual Meeting in Washington, D.C. From left to right: Yi Li (John Jay College of Criminal Justice of the City University of New York), Tim Kelley (North Carolina State University), and David E. Keyes (King Abdullah University of Science and Technology). Photo courtesy of James Crowley.

I am a computational scientist of mathematical origin from a time when computational science was not yet recognized. As a result, I had to grow into the field by starting over in multiple disciplines to learn applications, models, software, and hardware. Mathematics is a common thread and prerequisite.

I have co-originated and co-named two algorithms, both with Xiao-Chuan Cai (University of Colorado Boulder): (i) the Newton-Krylov-Schwarz algorithm, a domain-decomposed solver for nonlinear systems that arise in implicit discretizations of partial differential equations, and (ii) the Additive Schwarz preconditioned inexact Newton algorithm, a mostly asynchronous method for the same types of systems.

Like Tim Kelley (North Carolina State University), my colleague and fellow 2018 Fellow, I am heavily invested in Newton's method. In fact, our co-authored paper on pseudo-transient continuation for nonlinear systems is among our most highly-cited articles.

This brings me back to community. Mathematicians can work alone, and some do with great success. But they can enrich their problem space and enhance their creativity by seeking out the "pathologies" of others based on applications and stresses from computer hardware.

We stand today on the threshold of the convergence of the so-called third paradigm of large-scale simulation and fourth paradigm of big data. I look forward to this convergence, as it will expand community as well as extend the imaginations and central importance of mathematicians.

David E. Keyes is a professor of applied mathematics and computational science, as well as director of the Extreme Computing Research Center at KAUST.

Math Modeling

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Interestingly, one year I had a team of eager precalculus students participate in HiMCM alongside my high-level modeling students; they outperformed half of the modeling class, proving that math level is not a barrier to the modeling process.

Student Reflections on Modeling

A student enrolled in my modeling course this year after experiencing a great deal of math anxiety in previous math classes. He has become so passionate about modeling that he applied for—and received—a college scholarship for computational modeling. He is currently participating in a school trip to China focused on computational modeling and artificial intelligence.

High school modeling experience has motivated a number of strong math students to pursue computational mathematics. Even those who have followed other paths voiced their appreciation of exposure to modeling's collaborative and iterative nature. "When minds can collaborate, we realize possibilities that we wouldn't have thought of before," said one student. "I think it's good to learn to work together towards solving a problem and present the solution in a polished manner."

References

[1] *Guidelines for Assessment and Instruction in Mathematical Modeling Education*. (2019, February). (2nd ed.). Philadelphia, PA: Society for Industrial and Applied Mathematics and Consortium for Mathematics and Its Applications.

Greta Mills is a mathematics teacher and chair of the Mathematics Department at Oxbridge Academy in West Palm Beach, Fla.


Students in Greta Mills' honors seminar on math modeling at Oxbridge Academy participate in the 2017 High School Mathematical Contest in Modeling. The students designed a mountain resort that could serve as the location for a future Winter Olympic Games. Photo courtesy of Oxbridge Communications.