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Deep Learning for COVID-19 Diagnosis

By Keegan Lensink, William Parker, and Eldad Haber

Over the last several months, the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has rapidly become a global pandemic, resulting in nearly 480,000 COVID-19 related deaths as of June 25, 2020 [6]. While the disease can manifest in a variety of ways—ranging from asymptomatic conditions or flu-like symptoms to acute respiratory distress syndrome—the most common presentation associated with morbidity and mortality is the presence of opacities and consolidation in a patient's lungs. Upon inhalation, the virus attacks and inhibits the lungs' alveoli, which are responsible for oxygen exchange. In response—and as part of the inflammatory repair process—the alveoli fill with fluid, causing various forms of opacification within the lungs. This opacification is visible on computed tomography (CT) scans. Due to their increased densities, these areas appear as partially opaque regions with increased attenuation, which is known as a ground-glass opacity (GGO). Consolidation occurs when the accumulation of fluid progresses to an opaque region on CT scans (see Figure 1).

As COVID-19 spreads, healthcare centers around the world are becoming overwhelmed and facing shortages of essential equipment that is necessary to manage the disease's symptoms. Severe cases often require admission to the intensive care unit (ICU) and necessitate mechanical ventilation, both of which have limited availability. Rapid screening is crucial in diagnosing COVID-19 and slowing its spread, and effective tools are essential for prognostication in order to efficiently allocate increased care to those who need it most.

While reverse transcription polymerase chain reaction (RT-PCR) has thus far been the gold standard for COVID-19 screening in many countries, equipment shortages and strict requirements for testing environments limit this test's utility in all settings. Furthermore, reports indicate that RT-PCR testing suffers from high false negative rates due to its relatively low sensitivity and high specificity [1]. Chest CT scans—which have demonstrated effectiveness in the diagnostic process, including follow-up assessment and evaluation of disease evolution—are an important complement to RT-PCR tests [7]. Recent work indicates that trained radiologists' analyses of chest CT scans enable highly sensitive diagnosis [1].

In addition to providing complimentary diagnostic properties, CT scans have proven invaluable for the prognostication of COVID-19 patients. The percentage of well-aerated lung (WAL) has emerged as a predictive metric for determining prognosis, including admission to the ICU and death [3]. Practitioners often quantify the percentage of WAL by visually estimating volume of opacification relative to healthy lung; one can approximate this automatically via attenuation values within the lung. In addition to the percentage of WAL—which does not account for the various forms of opacification—expert interpretation of CT

See **COVID-19 Diagnosis** *on page 4*

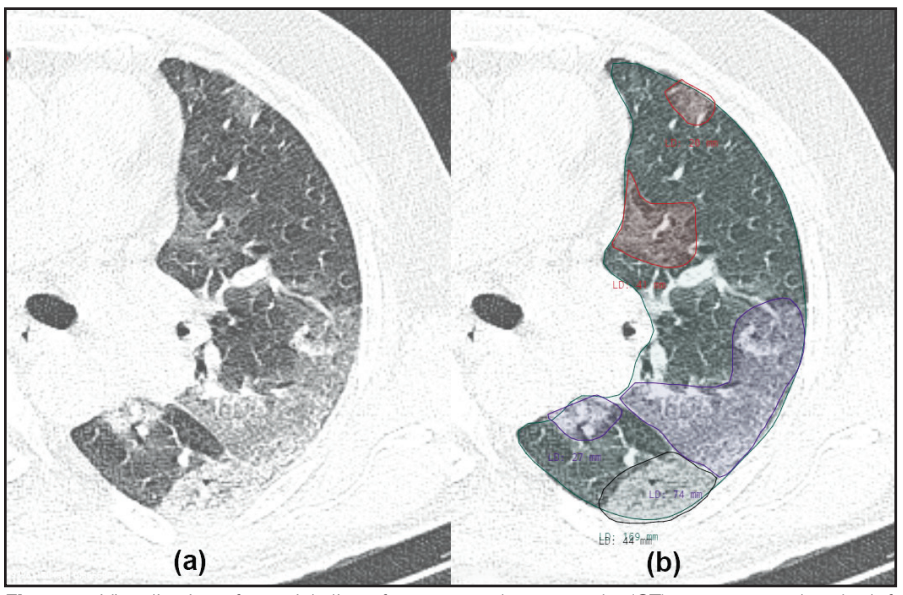

Figure 1. *Visualization of an axial slice of a computed tomography (CT) scan, cropped to the left lung.* **1a.** *Pulmonary opacification present in a patient with COVID-19.* **1b.** *The corresponding annotation generated by a radiologist. Red indicates pure ground-glass opacity (GGO), purple designates GGO with intralobular lines (crazy paving), and black signifies consolidation.*

Modeling Population Recovery Following an Environmental Disturbance

By Azmy S. Ackleh and Amy Veprauskas

What do populations of invasive and endangered species have in common? To find out, consider the following two contrasting scenarios.

Small mammals, such as kangaroo rats, are considered to be keystone species in many grassland and shrubland communities [7]. This means that their presence and densities help shape community composition. Because they are granivores, kangaroo rats significantly impact annual plants that serve as a resource base [4]. However, these communities are subject to various disturbances—including habitat fragmentation, fires, and livestock grazing—that degrade habitat quality and regularly threaten keystone species. For kangaroo rats, dense covers of herbaceous nonnative plants magnify the effects of these disruptions [5]. This type of vegetation cover has been shown to affect population recovery following a disturbance.

In contrast, American bullfrogs are an invasive species that damage native fauna in habitats around the world [8]. The bullfrog tadpoles' voracious appetites may dramatically reduce algae biomass—in turn reducing primary production and nutrient cycling—while adults compete with native species of birds, reptiles, amphibians, and fish for food sources [9]. As such, bullfrogs may have profound effects on native habitats, changing ecosystem structure and even causing local extinctions among native species. Control methods for American bullfrogs typically focus on the removal of tadpoles or adults from the population.

What similarities exist between these two scenarios? In addition to both populations substantially impacting overall community structure, these situations have two common components. Both cases involve the idea of a *disturbance* — such as habitat fragmentation or fires in the first case, or the intentional removal of individuals in the latter. There is also the concept of *recovery*. Recovery for an invasive species means that management strategies must be reapplied or modified. Recovery of an endangered species is the end goal.

Biological populations continually experience natural and anthropogenic disturbances—like hurricanes, fires, and chemical and noise pollution—that negatively influence their growth. From a management perspective, it is important to be able to quantify the way in which disturbances may affect a population's dynamics over time. This knowledge can help set harvest or land use regulations, identify effective conservation approaches, or aid in the establishment of control measures for pest species. However, one must exercise caution when applying management strategies; in some cases, they may have unintended effects. For instance, studies have shown that the aforementioned strategy for bullfrog regulation might be an ineffective means of population control, and in some cases actually result in increased population sizes. Instead, removal of metamorphs in the fall

See **Population Recovery** *on page 3*

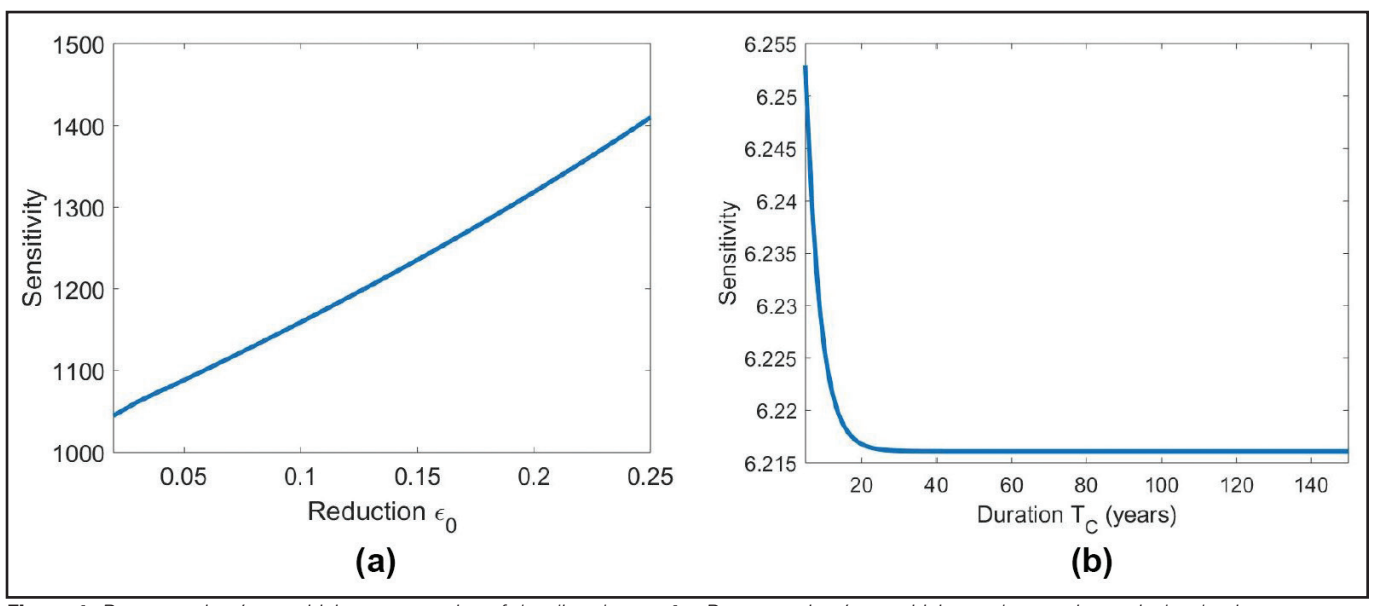

Figure 1. *Recovery time's sensitivity to properties of the disturbance.* **1a.** *Recovery time's sensitivity to changes in survival reduction ϵ_0, assuming a 10-year duration of impact.* **1b.** *Duration of impact T_C, assuming a five percent reduction in survival. Figure adapted from [1].*

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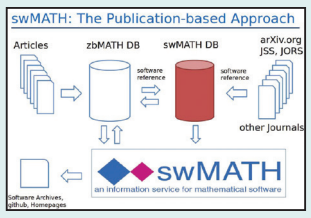

Broken Social Contract

LETTER TO THE EDITOR

The video of Mr. George Floyd dying on the street in Minneapolis, Minn., is almost too difficult to watch, yet its impact has been profound. Academia must reflect on this incident. Seven decades ago, universities began ramping up the research component of mathematics departments. Every year since, meager handfuls of minorities have obtained doctorates from mathematical sciences and statistics (MSS) departments. The mathematical aspirations of countless minorities have died in silence. No video recorded these deaths. When was the last time that you advised a Native American undergraduate or discussed mathematics with a Native American mathematician? Such a glaring lack of contact with this one important minority group is evidence of the harm inflicted by MSS departments on the minority population in general.

The current unrest that we see on the streets is connected to white privilege. I earned a Ph.D. in mathematics, which led me out of poverty and granted me privileges. I had a safe work environment, a regular paycheck, health insurance, and a retirement account. I traveled around the world and own a home. Few minorities have these privileges.

There is an implicit social contract between the minority community and MSS departments. The tax dollars of minorities support the research and privileges of faculty in MSS departments; in return, MSS departments educate minority children. That social contract has broken.

I call on our profession to recognize the professional privilege in which we live and reformulate departmental policies, attitudes, and programs of study with a view towards producing an equitable educational system for women, minorities, and all our citizens. How much longer must women and minorities call for change? Must we wait for calls to defund our MSS departments? On the other hand, will MSS departments take the lead in addressing reform?

This letter will also appear in MAA Focus, Notices of the AMS, the AWM Newsletter, and AMSTAT News.

— William Yslas Vélez, emeritus professor of mathematics at the University of Arizona

Obituary: Bernard J. Matkowsky

By Alvin Bayliss, Michael J. Miksis, and Vladimir A. Volpert

On June 11, 2020, our friend and colleague Bernard J. Matkowsky passed away. He was 80 years old. Bernie joined the faculty of Northwestern University's McCormick School of Engineering in 1977 and retired in 2018, having established a prestigious reputation at both the university and within the greater applied mathematics community.

Bernie graduated from the City College of New York in 1960 with a degree in electrical engineering. He proceeded to earn two master's degrees (in electrical engineering and mathematics) from New York University (NYU). Bernie received his Ph.D. in mathematics from NYU in 1966 under the direction of Joseph Keller. He then joined the faculty at Rensselaer Polytechnic Institute before eventually moving to Northwestern, where he remained for the rest of his career.

Bernard J. Matkowsky, 1939-2020. Photo courtesy of Alvin Bayliss.

Bernie made numerous major contributions to the field of applied mathematics. These developments include advances in asymptotic analysis of singularly perturbed problems, dynamical systems, stochastic differential equations, and pattern formation and scientific computation — despite his oft-stated remark that "gentlemen don't compute." In terms of application areas, he contributed significantly to combustion science and solid and fluid mechanics, among other disciplines.

Bernie's colleagues and peers regularly recognized him with honors too numerous to list in detail. These awards included a Fulbright-Hays Fellowship, a Guggenheim Fellowship, two medals from the Russian Academy of Sciences, and recognition as an Institute for Scientific Information Highly Cited Researcher. He was a Fellow of SIAM, the American Association for the Advancement of Science, and the American Physical Society. Bernie published more than 250 papers during his career. Upon his retirement from Northwestern, the Department presented him with bound copies of his complete papers, which extended to four thick volumes.

Bernie's service to Northwestern's Department of Engineering Sciences and Applied Mathematics—as well as the applied math community at large—was legendary. He served as department chair for six years, guiding the department through some challenging situations. Even after stepping down as chair, Bernie was an ever-present force, providing sound advice and support on a continuing basis.

Along with his colleagues Stephen Davis, Ed Olmstead, and the late Ed Reiss, Bernie helped build the department in the late 1970s and early 1980s; his duties included recruiting and mentoring the current senior faculty. Even while in ill health during his later years, Bernie never lost his devotion to the department and its faculty, and was always willing to provide advice and global perspectives. His unwavering focus on the application of math to real-world problems in science and engineering inspired a department that was unique for its time and has served—and continues to serve—as a model for other applied mathematics departments and programs around the country.

Outside of his department at Northwestern, Bernie remained an active member of SIAM. He served on the Editorial Board of the *SIAM Journal on Applied Mathematics* for 18 years (1977-1994), which included a stint as associate managing editor (1978-1982). He also acted as vice chair of the SIAM Activity Group on Dynamical Systems (1988-1990). In 2017, Bernie received SIAM's John von Neumann Prize and delivered the associated prize lecture at the 2017 SIAM Annual Meeting.[1]

Bernie was an outstanding advisor, mentor, and friend to his students, preparing them for successful careers in applied mathematics. He had a wide network of collaborators that reached Israel, Europe, and the former Soviet Union. In particular, Bernie recognized the rich heritage of theoretical combustion that was developed in the USSR. He was instrumental in disseminating this heritage in the U.S. via published papers and collaborations with eminent Soviet combustion theorists.

Bernie is survived by his wife Fraydie of 55 years, three children—David, Daniel, and Devorah—and six grandchildren. Those whose lives he touched will never forget him. His vision, energy, and devotion to applied mathematics, both at Northwestern and throughout the country, will remain a lasting legacy.

Alvin Bayliss, Michael J. Miksis, and Vladimir A. Volpert are professors in the Department of Engineering Sciences and Applied Mathematics at Northwestern University. All three interacted extensively with Bernard Matkowsky for many years.

[1] https://sinews.siam.org/Details-Page/singular-perturbations-in-noisy-dynamical-systems

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Solving Combinatorial Optimization Problems on Quantum Computers

By Yuri Alexeev, Jeffrey Larson, Sven Leyffer, and Ruslan Shaydulin

The rapid solution of combinatorial optimization problems benefits numerous applications. Quantum computing has recently attracted considerable attention due to numerous algorithms with exponential speedup over state-of-the-art classical algorithms. However, no demonstrably faster quantum algorithm currently exists for combinatorial optimization. The quantum approximation optimization algorithm (QAOA) is a candidate quantum algorithm for combinatorial optimization on gate-model quantum computers, such as those developed by IBM, Google, and Rigetti Computing. Here we overview the fundamentals, advantages, disadvantages, and current state of QAOA.

Edward Farhi and collaborators first introduced QAOA in 2014 to improve the best-known approximation ratio for a specific maximum satisfiability problem (Max E3LIN2) [2], though researchers have since developed a better classical algorithm. While QAOA has yet to theoretically improve upon the best classical algorithms for any problem class, it continues to attract interest within the quantum computing and optimization communities.

The reasons for this interest are twofold. QAOA is one of few algorithms that can reliably run on near-term quantum devices. QAOA and its generalization—the quantum alternating operator ansatz [4]—can also tackle a wide class of combinatorial optimization problems that are computationally difficult and ubiquitous in applied mathematics. To disentangle the hype from reality, we first recap the mathematics of quantum computation and QAOA. Consider the combinatorial optimization problem over the Boolean hypercube and its reformulation:

$$\min_{\mathbf{y}\in\{0,1\}^n} f(\mathbf{y}) \;\Leftrightarrow\; \min_{\mathbf{y}\in\{0,1\}^n} \sum_{\mathbf{w}\in\{0,1\}^n} f(\mathbf{w})\mathbb{1}_{\mathbf{w}}(\mathbf{y}), \tag{1}$$

where the second formulation is an equivalent representation of $f(\mathbf{y})$ and $\mathbb{1}_{\mathbf{w}}(\mathbf{y})$ is the indicator function that takes the value 1 if $\mathbf{w}=\mathbf{y}$ and 0 otherwise.[1] Note that construction of such an indicator polynomial is simple but might require 2^n terms in the sum.

This technique can convert the *objective function* f—which acts on the Boolean hypercube—into an *operator* $\hat{f}$ that acts on the 2^n-dimensional space $\mathbb{C}^{2^n}$ in the following way: $\hat{f}\cdot\mathbf{e}_i = f(\mathbf{y})\mathbf{e}_i \;\forall i$, where $\mathbf{e}_i\in\mathbb{C}^{2^n}$ is an element of an orthonormal basis $\{\mathbf{e}_i\}_{i=1}^{2^n}$ of $\mathbb{C}^{2^n}$ that encodes a binary string $\mathbf{y}\in\{0,1\}^n$. Because $\dim(\mathbb{C}^{2^n})=2^n$, one can use any basis of $\mathbb{C}^{2^n}$ to encode all binary strings $\mathbf{y}\in\{0,1\}^n$. We can construct $\hat{f}$ by replacing the indicator function $\mathbf{1}_{\mathbf{e}_i}(\mathbf{y})$ with the projector operator $\mathbf{e}_i(\mathbf{e}_i^*)^T$, where $\mathbf{e}_i^*$ denotes the complex conjugate of $\mathbf{e}_i$. Since $\{\mathbf{e}_i\}_{i=1}^{2^n}$ is an orthonormal basis, this projector behaves like the indicator function: $\mathbf{e}_i(\mathbf{e}_i^*)^T\mathbf{e}_j=\mathbf{e}_j$ if $i=j$ (operator acts as identity) and is otherwise 0. While illustrative, this view does not provide a recipe for efficient construction of $\hat{f}$ for a given f. A comprehensive list of rules on constructing operators $\hat{f}$ is available in [3].

We now connect the combinatorial optimization problem to a quantum computer. We represent the state of an n-qubit quantum computer with a norm-1 vector in $\mathbb{C}^{2^n}$. By selecting the basis in $\mathbb{C}^{2^n}$ to embody all binary strings $\mathbf{y}\in\{0,1\}^n$, we can convert our cost function into a *quantum operator* that acts on a quantum computer's state space. Note that this operator is simply a diagonal matrix. QAOA considers the following family of parameterized vectors:

$$\mathbf{x}(\beta,\gamma)=\prod_{i=1}^{p}(e^{-i\beta_i\hat{m}}e^{-i\gamma_i\hat{f}})\mathbb{1}\in\mathbb{C}^{2^n},$$

where $p\in\mathbb{N}$, $\beta\in[0,\pi]^p$, $\gamma\in[0,2\pi]^p$ are free parameters, and $\mathbb{1}=\frac{1}{2^n}\sum_i\mathbf{e}_i$. The mixing operator $\hat{m}$ is a nondiagonal matrix that "mixes together" terms that correspond to different basis vectors. Researchers typically employ a "transverse field" operator as the mixing operator [4].

See **Quantum Computers** *on page 6*

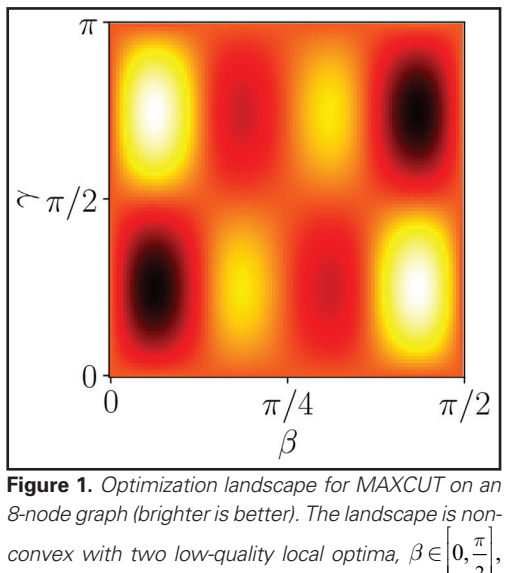

Figure 1. *Optimization landscape for MAXCUT on an 8-node graph (brighter is better). The landscape is non-convex with two low-quality local optima, $\beta\in\left[0,\frac{\pi}{2}\right]$, $\gamma\in[0,\pi]$. Figure courtesy of Ruslan Shaydulin.*

[1] This representation is a version of the *Fourier expansion* of f. Further discussion of Fourier analysis of Boolean functions is available in [7].

Population Recovery

Continued from page 1

may be more effective [8]. And while livestock grazing is generally believed to negatively impact some species' environments, research has indicated that it can actually promote kangaroo rat recovery if it reduces vegetation coverage [6].

Mathematical modeling can serve as a complementary tool to experimental studies for understanding the implications of management or control strategies. It is both inexpensive and able to provide real-time management methods that do not require extended periods of data collection. However, model predictions rely heavily on the data's accuracy and the assumptions used in model development. Nevertheless, models can provide useful insights—even when limited data is available—and help generate hypotheses that inform experimental designs. Here we present a general modeling approach for the study of population recovery. This approach is adaptable to various situations and may assist in the identification of effective control strategies.

How Can We Model Recovery?

Depending on the population under consideration, a population's recovery may take many forms. If we wish to mathematically model recovery, we must first define the way in which a population's size changes over time. To do so, we describe a population using a matrix model that allows us to distinguish between individuals in different developmental stages.

Consider a female population that is divided into m stages. Denote the densities of these stages at time t with $\mathbf{n}(t):=[n_1(t),n_2(t),\ldots,n_m(t)]^\intercal$, where $\intercal$ signifies the transpose of a vector. Let $\mathbf{A}[\boldsymbol{\theta}(\epsilon(t),\mathbf{n}(t)),\epsilon(t)]$ be the projection matrix for the population at time t that describes individuals' transitions between the different stages. This matrix is dependent on the environment at time t—as described by $\epsilon(t)$—as well as the vital rates that are realized by this environment and the current population density $\boldsymbol{\theta}(\epsilon(t),\mathbf{n}(t))$. The matrix model determines the population at the next time step:

$$\mathbf{n}(t+1)=\mathbf{A}[\boldsymbol{\theta}(\epsilon(t),\mathbf{n}(t)),\epsilon(t)]\mathbf{n}(t),\quad t=0,1,2,\ldots. \tag{1}$$

We use ϵ to describe the proportional reductions in vital rates that result from an environmental disturbance.

We can define population recovery as occurring when the total population reaches a designated threshold N_{rec}, such as the population's carrying capacity or size prior to the disturbance. If we assume that a disturbance transpires at time $t=0$, the recovery time will be the smallest integer solution to

$$\prod_{i=0}^{t}\mathbf{A}[\boldsymbol{\theta}(\epsilon(i),\mathbf{n}(i)),\epsilon(i)]\mathbf{n}(0)\geq N_{rec}. \tag{2}$$

The simplest way to describe a disturbance is with a step function, which dictates that the effects of a disturbance are either "on," $\epsilon(t)=\epsilon_0$, or "off," $\epsilon(t)=0$. If we assume that the environment follows a step function and population growth is independent of density (as may be appropriate for endangered populations), the recovery time becomes the solution to the equation

$$\mathbf{1}_m^\intercal\mathbf{A}_0^{t-T_C}\mathbf{A}_{\epsilon_0}^{T_C}\mathbf{n}(0)=N_{rec}, \tag{3}$$

where $\mathbf{1}_m$ is a $m\times 1$ vector of ones.

How Sensitive are Recovery Predictions?

Sensitivity analysis measures the way in which small perturbations in a model parameter affect model output. When examining a population's recovery, the recovery time's sensitivity to a model input can help identify the most effective management or control strategy. One can calculate sensitivity in its simplest form just by taking a derivative. Using (3) to model recovery, we can find the recovery time's sensitivity by implicitly differentiating this equation. For instance, the sensitivity of the recovery time with respect to the magnitude of impact is given by

$$\frac{dT_{rec}}{d\epsilon_0}=-\frac{\mathbf{1}_m^\intercal\mathbf{A}_0^{T_{rec}-T_C}(\mathbf{n}(0)^\intercal\otimes\mathbf{I}_m)}{(\mathbf{A}_{\epsilon_0}^{T_C}\mathbf{n}(0))^\intercal(\mathbf{I}_m\otimes\mathbf{1}_m^\intercal\mathbf{A}_0^{-T_C})}\times\frac{\frac{d(\mathbf{A}_{\epsilon_0}^{T_C})}{d\mathbf{A}_{\epsilon_0}}\frac{d\,\mathrm{vec}[\mathbf{A}_{\epsilon_0}]}{d\epsilon_0}}{\frac{d\,\mathrm{vec}[\mathbf{A}_0^{T_{rec}}]}{dT_{rec}}}, \tag{4}$$

where the $\otimes$ operator denotes the Kronecker product and the vec operator converts a matrix into a column vector by stacking the matrix's columns. In a similar manner, we can also use (3) to derive sensitivity formulas of the recovery time with respect to a vital rate or the initial population distribution [1].

To illustrate the utility of equations such as (4), we present an application that investigates the recovery of sperm whales, which are impacted by a variety of disturbances that include oil spills and noise pollution. We use a discrete-time stage-structured model to examine a sperm whale population [3]. In Figure 1 (on page 1), we present the recovery time's sensitivity for a sperm whale population with respect to changes in the magnitude of impact ϵ_0 and duration of impact T_C. These graphs indicate that the recovery time is more sensitive to changes in ϵ_0 than T_C. For instance, consider the effect of a 20 percent increase in these two parameters. If $\epsilon_0=0.20$, a 20 percent increase in ϵ_0 heightens survival reductions from 20 to 24 percent, resulting in an additional 53 years of recovery time. In contrast, when we consider the recovery time's sensitivity to changes in the duration of impact, this graph approaches a value close to six. Therefore, each additional year of impact increases the recovery time by approximately six years. If we thus increase T_C from 10 to 12 years (a 20 percent increase), the recovery time is only extended by 12 years.

Graphs such as Figure 1 (on page 1) provide important insights into a population's recovery and management following a disturbance. In the context of sperm whales, Figure 1 suggests that conservation efforts should focus on reducing the magnitude of impact rather than the duration. In the case of a contaminant spill such as oil, this type of mitigation might include strategies that focus on removing the contaminant from the water. Similar analysis also indicates that management should concentrate on the mature individuals. As illustrated by this example, our model framework may provide useful insights even when limited data is available.

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COVID-19 Diagnosis

Continued from page 1

scans provides insight into an infection's severity by identifying numerous patterns of opacification (see Figure 2).

The prevalence of these patterns, which correlate with the severity of infection, are associated with different stages of COVID-19. Quantification of both the WAL percentage and the opacification composition enables efficient estimation of the disease's stage and potential patient outcome.

Radiologists typically analyze three-dimensional (3D) images. However, 3D quantitative assessment is both difficult and time consuming. Computerized techniques—particularly machine learning methods that are based on deep convolutional neural networks (CNNs)—can aid in this endeavor.

Researchers have widely applied deep learning-based methods in vision. These methods are based on a simple model:

$$\mathbf{Y}_{j+1} = F(\mathbf{Y}_j, \boldsymbol{\theta}_j), \quad j = 1,\ldots,n,$$

where $\mathbf{Y}_j$ specifies hidden layers, $\mathbf{Y}_1$ is the original 3D image, and the function F (which depends on the parameters $\boldsymbol{\theta}$) is typically composed of convolutions and a nonlinear activation function. One of the most successful architectures in recent years employed a function of the form $F(\mathbf{Y}_j, \boldsymbol{\theta}_j) = \mathbf{Y}_j + G(\mathbf{Y}_j, \boldsymbol{\theta}_j)$. This architecture, called a residual method, is linked to the discretization of the ordinary differential equation (ODE) [4]:

$$\dot{\mathbf{Y}} = G(\mathbf{Y}, \boldsymbol{\theta}).$$

In recent years, scientists have used such networks in medical imaging; several groups are now utilizing them to combat COVID-19. Although researchers have proposed plenty of artificial intelligence (AI) systems to provide assistance with the diagnosis of COVID-19 in clinical practice, AI has not yet shown any significant impact in improving clinical outcomes.

As part of a project that is spearheaded by Vancouver General Hospital, we aim to improve the clinical diagnosis—and particularly the prognosis—of COVID-19. We are combining advanced machine learning algorithms with annotated CT scans to develop a *quantitative diagnostic tool* that can help physicians diagnose and manage COVID-19 patients. Similar to other undertakings, the basic idea involves using annotated images and then training a deep learning network that can automatically classify areas on the 3D CT scan based on their type. Assuming that this can be done successfully, one can estimate the different labels' volumes—in addition to the percent WAL—and correlate them to clinical outcomes. This approach thus allows practitioners to not only diagnose COVID-19 patients (which radiologists can do relatively easily), but also provide quantitative analyses that predict outcomes.

Data is one of the most important aspects of such a project. We were fortunate to obtain nearly 5,000 CT images from Iran; China; South Korea; Italy; Saudi Arabia; and Vancouver, Canada. Volunteer physicians in Vancouver then annotated this data, obtaining a large and diverse dataset for training, validating, and testing.

Although we initially imagined working with fairly standard networks and optimization routines for segmentation, we quickly encountered two main problems. The first issue is the variability between physicians in terms of the "correct" segmentation. Our images are very different from classical machine learning applications — such as the segmentation of objects on a street, wherein a nonexpert can easily identify the classes. In one of our first studies, 12 physicians segmented the same image. The results varied significantly (see Figure 3).

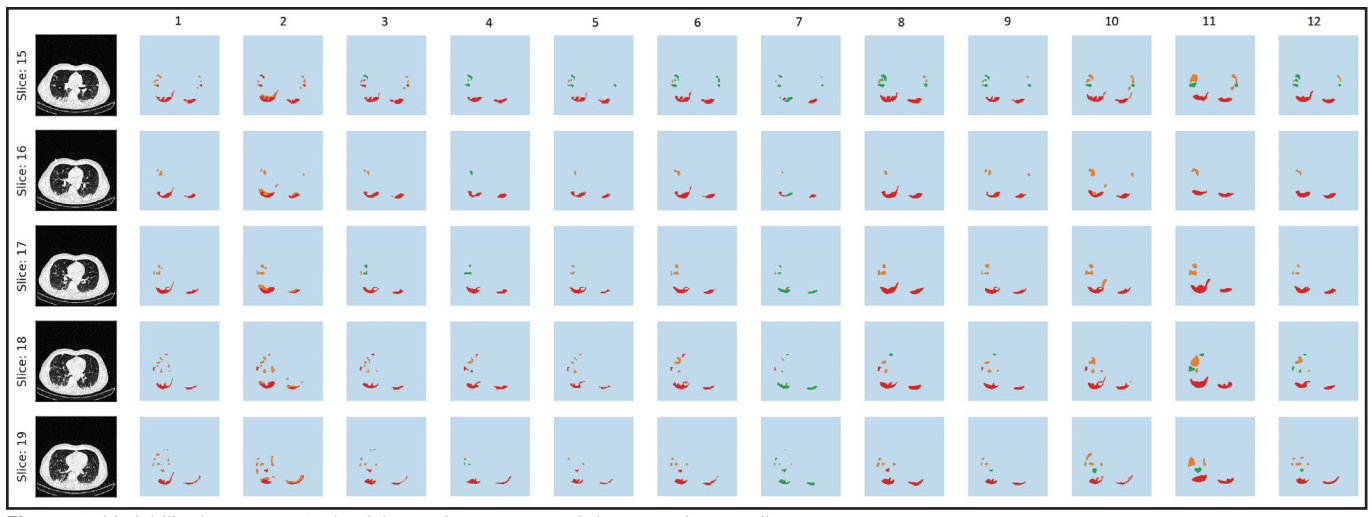

Figure 3. *Variability between 12 physicians who segmented the same image slices.*

This variability implies that it is misguided to use simple objective functions (like cross entropy) that are common in deep learning to guide the optimization process. It also indicates that utilization of well-known metrics, such as Intersection Over Unions, to check the segmentation's quality is misguided as well. To handle the variability, we developed a noise model and included it in the optimization process. Creation of this model and its subsequent involvement in training procedures was a main goal in our effort to ensure that the results were meaningful for clinical use.

The size and dimension of the problem presented a second bottleneck. Unlike most image analysis problems, CT is typically collected in three dimensions and presents 3D targets. True comprehension of a CT image's clinical implication requires a 3D understanding of structures. Previous researchers have employed 3D CNNs, mainly for video. However, these networks—especially when deep—tend to require a large amount of memory. This complication makes it impossible to train a deep network in three dimensions without special hardware. In response, and inspired by hyperbolic partial differential equations, we developed hyperbolic neural networks that necessitate a fixed amount of storage — a fraction of the storage required when training typical networks [2, 5]. These hyperbolic networks allow us to train deep networks on high-resolution 3D images. They are based on the leapfrog discretization of the second-order ODE,

$$\ddot{\mathbf{Y}} = G(\mathbf{Y}, \boldsymbol{\theta}),$$

and rely on the properties of hyperbolic systems that move forward and backward in time. This permits us to train deep neural networks on modest hardware.

Vancouver General Hospital is currently validating the results of our research, which will soon be released as open software.[1] Ultimately, we hope to provide radiologists around the world with better tools for the diagnosis and prognosis of COVID-19 patients.

[1] https://github.com/UBC-CIC/COVID19-L3-Net

Pattern Description	Class Number	Group Number
Background	0	0
Left Lung	1	1
Right Lung	2	1
Pleural Effusion	3	0
Lymphadenopathy	4	0
Pure Ground Glass Opacification	5	2
GGO w/ Smooth Interlobular Septal Thickening	6	3
GGO w/ Intralobular Lines (Crazy Paving)	7	3
Organizing Pneumonia Pattern	8	4
GGO w/ Peripheral Consolidation (Atoll Sign)	9	4
Consolidation	10	4

Figure 2. *Classes annotated in the dataset, as well as the class groupings we utilized in our experiments.*

This work is based on Eldad Haber's minitutorial presentation as part of the 2020 SIAM Conference on Mathematics of Data Science (MDS20), which occurred virtually in May and June. Haber's presentation is availabe on SIAM's YouTube channel.[2]

The figures in this article were generated by the authors.

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[2] https://www.youtube.com/watch?v=jGCLyjv4bbk

The Mathematics of Mass Testing for COVID-19

By David Donoho, Mahsa Lotfi, and Batu Ozturkler

Nobel Prize-winning economist Paul Romer views the global COVID-19 shutdown as an economic calamity. Trillions of dollars of economic losses fell on individuals, businesses, and governments; these losses will become permanent if society does not soon resume pre-virus activities. Romer, who previously served as Chief Economist of the World Bank, proposes a confidence-inspiring path out of the shutdown based on dramatically expanded COVID-19 testing. He indicates that everyone in the U.S. should get tested every two weeks. Those who test positive should self-isolate while the rest of the economy reopens, enabling new jobs and investments.[1] Romer's simulations reveal that this technique will keep the population's active infection rate below five percent, ensure that most people do not get infected, and spur rapid economic recovery.

Unfortunately, we currently cannot possibly test at the levels Romer envisions, which involves screening seven percent of the population every day. For context, only about four percent of U.S. residents were tested for COVID-19 from March through May.

Inspired by the call for a dramatic scale-up of testing, statistician David Donoho reviewed a recently emergent research front in which mathematical and statistical ideas—implemented through data science—can enable a rapid expansion of testing capabilities worldwide. He surveyed this new front during an invited presentation at the inaugural 2020 SIAM Conference on Mathematics of Data Science (MDS20),[2] which occurred virtually in May and June, in hopes that the SIAM community would contribute to novel research trends related to COVID-19.

Such trends continue to come together in part due to the new medRxiv preprint server for health sciences. Mathematical scientists have enjoyed the arXiv preprint service for nearly 30 years and are accustomed to sharing information universally, rapidly, and freely. However, medical literature was always restricted and paywalled. In 2019, medRxiv was founded as an offshoot of bioRxiv to provide the capability for globally visible medical research preprint literature.

The COVID-19 crisis brought medRxiv to life. A stream of COVID-19 postings began in January 2020; by March, hundreds of items were flooding in daily. Submissions covered everything from individual case reports and documentation of care protocols to fully-developed articles about therapeutic interventions intended for major journals. Contributors included doctors sharing patient data, medical teams conducting clinical trials, public health officials analyzing national databanks, medical device engineers discussing new technologies, and citizen scientists focusing on COVID-19 during lockdown.

Several of these articles addressed the need to scale up testing efforts. Many papers sought to show that one could repurpose existing COVID-19 test kits in a multiplexed fashion, resulting in a substantial expansion of the total patient caseload under screening without increasing the number of testing stations or utilizing extra test kits.

During his talk, Donoho spotlighted two early papers in this burgeoning literature. One paper multiplexed patient samples up to five at a time in an organized protocol that immediately expanded effective testing capacity—the number of patients whose disease status can be determined—by more than a factor of two [1, 2]. Another submission suggested that much more was possible [7]. This paper documented the ability to multiplex up to 64 patient samples at a time and still detect the presence of COVID-19 in one individual patient. In principle, a single quantitative reverse transcription polymerase chain reaction (RT-qPCR) run on a pooled sample thus determines whether anyone among a group of 64 patients has the disease.

One principle is common to papers in this emergent research front: most people are not actually infected during population-level testing, so they will not have the active virus in their test samples. Intuitively, we do not really need to consume one test kit per patient if so few patients are actually infected. Instead, we need both multiplexing and math (see Figure 1).

Formally speaking, a test measures a sample's viral load. If we consider a group of N patients, the vector $\mathbf{x}$ of N viral loads will be sparse (mostly zeros) because the majority of people are not infected. Mathematically, the problem thus seeks to most efficiently—i.e., with fewest test kits and the least possible wall-clock-time delay—determine which entries are nonzero in a large, sparse vector of viral counts.

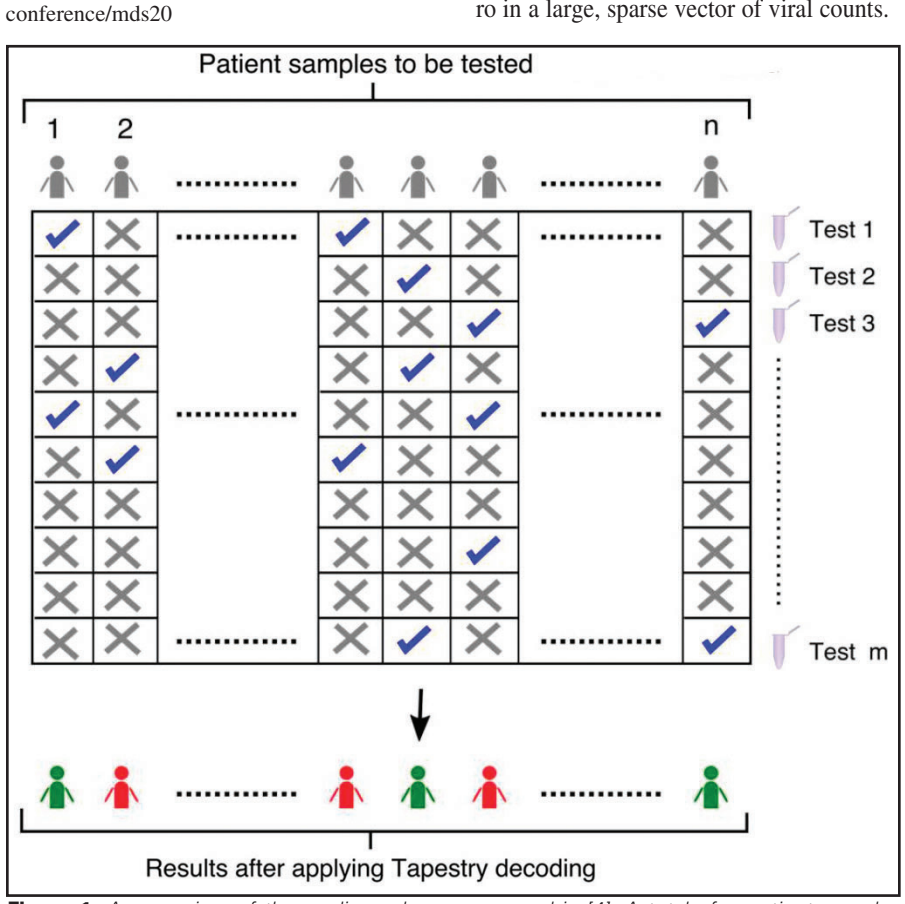

Figure 1. *An overview of the pooling scheme proposed in [4]. A total of n patient samples are pooled into m tests in a combinatorial manner. Each patient sample is included in multiple tests and each test contains multiple patient samples. Figure courtesy of [4].*

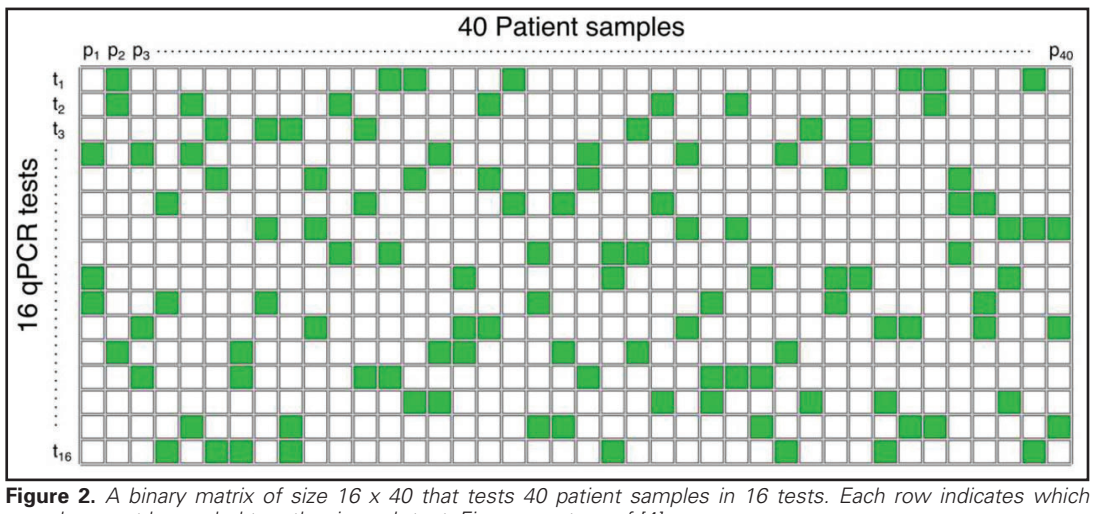

Figure 2. *A binary matrix of size 16 x 40 that tests 40 patient samples in 16 tests. Each row indicates which samples must be pooled together in each test. Figure courtesy of [4].*

Multiplexing involves pooling samples from several patients, wherein each patient's sample appears in multiple pools and each pool contains samples from multiple patients (see Figure 2). The total viral load in each test sample is roughly the sum of the viral loads contributed by every sample in that pool. One can collect the viral loads that underly T tests into a T by 1 vector $\mathbf{y}$. The tested viral loads $\mathbf{y}$ are related to the original viral loads $\mathbf{x}$ via matrix multiplication $\mathbf{y}=A\mathbf{x}$, where A is a T by N binary matrix that indicates which patients' samples contribute to which test pools. Now the problem involves inferring the sparse vector $\mathbf{x}$ from (noisy, partial, binary, and linear) information about $\mathbf{y}$. Researchers sometimes employ multiple rounds of measurement $\mathbf{y}_r=A_r\mathbf{x},\ r=1,\ldots,R$, with round r's pooling matrix A_r dependent on the last round's test results $\mathbf{y}_{r-1}$. One can then infer $\mathbf{x}$ from $\mathbf{y}=[\mathbf{y}_1,\mathbf{y}_2,\ldots,\mathbf{y}_R]$, once again obeying $\mathbf{y}=A\mathbf{x}$ — now with block matrix $A=\oplus_{r=1}^{R}A_r$. Scientists can build matrix A with appropriate use of randomness or delicate constructions that involve special bipartite graphs, special structured matrices, or even information-theoretic codes.

Eventually, one deciphers the test results $\mathbf{y}$ to determine which samples must contain the COVID-19 virus. The key point is that the total number of tests $T<N$, so practitioners are using T test kits to evaluate the disease status of N patients.

Deciphering the medRxiv proposals exploits knowledge of the instance data $(A,\mathbf{y})$ and assumed sparsity of $\mathbf{x}$. These papers are motivated by many techniques with which the SIAM community is familiar, including sequential approaches such as group testing or combinatorial group testing and one-round approaches inspired by compressed sensing and one-bit compressed sensing.

Donoho overviewed the basic RT-qPCR test—the gold standard of COVID-19 testing efforts—and explained why this technology could pair well with multiplexed samples. He also highlighted several additional research efforts that explicitly made the connection to mathematical sciences. For example, one team utilized combinatorial group testing [3, 5] and another employed compressed sensing [4]. Both techniques propose one-round-only methods and show—as in [6]—that they can successfully infer the disease status of N patients from T tests at low levels of population prevalence, where

$$N\approx 10T. \qquad (1)$$

When successful, this marks a tenfold expansion in the number N of patients whose disease states can be determined for the same number T of units of RT-qPCR machine time and test kits (N patient samples and the associated per-patient processing are of course still required). This approach would naturally require a very low prevalence of infection; however, N can be significantly larger than T even at a higher prevalence. A nice benefit of these two methods is that they are one-round-only $(R=1)$, so they experience less processing delay than multi-round procedures — a fact that patients will certainly appreciate.

Donoho was floored by the rapidity with which this research front developed, producing in mere weeks not only fascinating proposals and ideas but actual protocols for daily use. To close his MDS20 talk, he looked beyond today's RT-qPCR standard for COVID-19 testing and discussed some new technologies that may soon arrive. The need to dramatically increase global testing is clear, and the exuberant growth of new research fronts—combined with key mathematics-based enabling technology—inspires hope for future testing endeavors.

This article is based on David Donoho's invited presentation as part of the 2020 SIAM Conference on Mathematics of Data Science (MDS20), which occurred virtually in May and June. Donoho's presentation is availabe on SIAM's YouTube channel.[3]

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[1] https://paulromer.net/roadmap-to-reopen-america

[2] https://www.siam.org/conferences/cm/conference/mds20

[3] https://www.youtube.com/watch?v=VOzl-RC4IIs

Chaos (and Dynamics) for All!

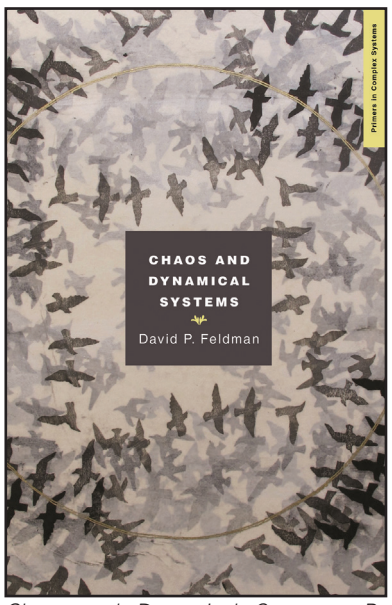
Chaos and Dynamical Systems. *By David P. Feldman. In Primers in Complex Systems. Princeton University Press, Princeton, NJ, August 2019. 264 pages, $35.00.*

BOOK REVIEW
By Lora Billings

While the field of dynamical systems continues to evolve, thus remaining true to its inherent definition, mathematicians' efforts to utilize these concepts to understand order and disorder are unwavering. David P. Feldman's new book, *Chaos and Dynamical Systems*, serves as an introduction to the field and falls somewhere between popular overviews on chaos theory and high-level textbooks on dynamics. His thoughtful approach engages readers at a variety of levels and draws them into the subject's distinct beauty.

Feldman offers simple, clear explanations that give meaning to his equations and figures and provide deeper insight for those in search of more detail. The book expects readers to be comfortable with algebra and functions, but goes light on calculus. Its readability and careful build-up to more advanced topics avoids an abstract leap that befalls many other texts in this field. *Chaos and Dynamical Systems* is therefore appropriate for an both undergraduate survey course or a graduate course that covers the broader theme of applied mathematics. Even experts would likely find it to be a nice addition to their libraries.

Feldman addresses modeling in both discrete and continuous dynamical systems, more commonly known as iterated functions and ordinary differential equations. The models are openly motivated as qualitative and intended to be descriptive or empirical, and he evidently chooses each chapter's classic examples based on their lucidity in standard analysis techniques. Not all simple models behave simply, and Feldman uses chapter three—entitled "Interlude: Mathematical Models and the Newtonian Worldview"—to philosophically discuss why researchers should optimistically continue to believe that the world is understandable. The subsequent two chapters introduce the concept of chaos, and Feldman writes that "Mathematical chaos is exquisitely lawful; a chaotic dynamical system obediently follows a deterministic rule in perpetuity." He also admits that students are often disappointed by this notion, as they frequently expect something weirder or stranger. Nevertheless, Feldman continues with interesting analyses of the butterfly effect, Lyapunov exponents, and symbolic dynamics, among other topics.



Chaos and Dynamical Systems. By David P. Feldman. Courtesy of Princeton University Press.

Feldman's discussion of bifurcations in chapter six is a fascinating journey that "connects the dots" for the reader, so to speak. Using an example that pertains to population dynamics, he demonstrates a bifurcation with discourse, equations, and figures. The end of the chapter explores a broader history of bifurcation theory and its connection to the popular concept of tipping points, complete with numerous suggestions for further reading.

Chapter seven tackles universality in chaos, which Feldman describes as "one of the most amazing results to emerge from the study of dynamical systems." Appropriately, researchers can employ the logistic function to introduce orbits, state diagrams, and bifurcation diagrams (which provide endless structure for investigation). Feldman then uses Feigenbaum's constant and period doubling to extend abstract concepts to real-world experimental observations. This process yields a general overview that touches on operators, critical transitions, renormalization, and applications in other physical systems.

Chapter eight turns to the classic Lotka-Volterra predator-prey model and the Rössler equations to introduce phase space and the chaos-related phenomena that are only visible in higher dimensional continuous systems. Feldman then utilizes Poincaré sections and delay coordinates to explore strange attractors in chapter nine. Although he only briefly touches on this incredibly rich subject, the suggestions for further reading in synchronization are excellent.

It is worth noting that *Chaos and Dynamical Systems* includes a few less traditional topics in dynamics, such as power laws and universality. Feldman concludes with a discussion of the spectrum of opinions on complex systems and emergence. He admits that the fields of complex and dynamical systems are inherently interdisciplinary, and believes that the different approaches keep them vibrant and appealing. Feldman's enthusiasm for the subject is contagious, and anyone who picks up his book will surely be engaged. After all, how many math books actually describe the discovery of emergent phenomena as exciting and fun?

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Quantum Computers

Continued from page 3

We use a classical optimizer to vary the free parameters β,γ and bring $\mathbf{x}(\beta,\gamma)$ as close as possible to the basis vector $\mathbf{e}_i$ that encodes the binary string $\mathbf{y} \in \{0,1\}^n$, which is the original problem's solution. We have thus replaced the combinatorial optimization over $\mathbf{y}$ with a nonconvex optimization over β,γ. Figure 1 (on page 3) illustrates the objective landscape. One can read the optimization result from the quantum computer by performing a measurement, which is equivalent to sampling from a probability distribution; when measuring vector $\mathbf{x}(\beta,\gamma)$, the result is $\mathbf{e}_i$ with the probability $|(\mathbf{e}_i^*)^T \mathbf{x}(\beta,\gamma)|^2$. If $\mathbf{x}(\beta,\gamma)=\mathbf{e}_i$, the measurement result will be $\mathbf{e}_i$ with probability 1.

Research has shown that one cannot efficiently sample from the output of QAOA under reasonable complexity theory assumptions, even with only one step ($p=1$). However, the fact that QAOA is classically hard to simulate does not speak to its potential for solving optimization problems. Nevertheless, a number of obstacles prevent people from *understanding* and *realizing* its potential, defined as the approximation ratios that it can achieve.

First, the following elements impede the ability to *understand* QAOA's potential:

(i) the lack of analytical results about QAOA behavior in depths other than $p=1$ or $p=\infty$

(ii) the lack of empirical results about QAOA scaling with problem size and QAOA performance on problems of realistic size.

Second, the subsequent factors hinder the *realization* of QAOA's potential (i.e., achieving quantum advantage through optimization):

(i) the need for parameter optimization (i.e., optimizing over β,γ)

(ii) the mismatch between the capabilities of available hardware and QAOA's hardware requirements, in terms of the number of qubits, speed, and fidelity of gates.

QAOA's potential is difficult to analyze in general, but two recent results provide analytical upper bounds on QAOA performance. Matthew Hastings demonstrated that classical local one-step algorithms achieve the same (or better) performance for $p=1$ as one-step QAOA [5]. Another group analyzed QAOA's locality and symmetry—with the practical corollary that the classical Goemans-Williamson algorithm for MAXCUT outperforms it in constant depth (i.e., constant p)—and provided an upper bound for arbitrary p [1]. While these results are interesting, a near-term potential of QAOA is its use as a heuristic. In this case, the worst-case QAOA performance may not predict its average-case performance. Unfortunately, QAOA's average-case analysis is impeded by its analytical complexity and the impossibility of numerical experiments for problems of nontrivial size, due to the lack of appropriately capable hardware and the computational cost of classical simulation. The greatest potential for better understanding lies at this point.

The dearth of methods to reliably and efficiently solve the parameter optimization within each QAOA iteration severely limits the *realization* of its potential. Any given problem and depth has no *a priori* knowledge of the parameter values β and γ that result in the distribution $\mathbf{x}(\beta,\gamma)$ that maximizes f. We must therefore search for these values, often with classical numerical optimization routines. While the optimization appears to be simple in higher depths ($p>n$) and is trivial in the limit $p\to\infty$, QAOA's most promising regime is shallow (small constant) depth because it can run on near-term hardware. For small depth, the objective over β and γ is often nonconvex and contains many poor local optima. Figure 1 (on page 3) is an example objective landscape in the $p=1$ case.

QAOA's performance depends critically on the quality of the parameters β and γ. However, a single local optimization run is the current default in multiple QAOA packages, even though the objective has many suboptimal local optima. One can gain considerable improvement via multistart optimization methods [9] or machine learning approaches [6], yet these techniques also struggle when p is a moderate size. The best numerical optimization routine for identifying parameters within QAOA is largely an open question.

The second limiting consideration is the required large number of qubits and fast, high-fidelity gates to execute QAOA circuits with $p \gg 1$. Classical algorithms can achieve excellent approximation ratios in minutes—if not seconds—for most practically interesting binary optimization problems with less than a few hundred variables. Therefore, until quantum hardware with hundreds of qubits is accessible, QAOA will not be able to compete with classical state-of-the-art methods under the current approach. Such devices may become available in the next several years. Hardware size is growing steadily, but simply increasing the qubit count is not enough. As QAOA gate count requirements grow linearly with the problem description and depth p, they quickly surpass current hardware's capabilities.

For example, QAOA requires execution of $d \times n \times p$ 2-qubit gates for MAXCUT on a d-regular graph on n nodes with depth p (assuming full connectivity between qubits and "controlled NOT" as the native 2-qubit gate). This in turn necessitates the execution of hundreds of 2-qubit gates for moderate-sized problems, which is beyond the capacity of existing hardware.

In our opinion, ion-trap architectures are one of the most promising near-term quantum computers for faithful execution of QAOA circuits due to the high fidelity of gates — albeit at low frequency. Several researchers have demonstrated QAOA simulations with 40 qubits and depth $p=1$ and $p=2$ [8]. They found that increasing $p=2$ did not improve the solution's quality because the error that resulted from the execution of extra gates negated any benefits. These results underpin the importance of high-fidelity quantum hardware to make significant progress. We hope that the ion trap and other technologies will improve in the midterm. Such advances will allow for large-scale evaluations of quantum optimization in realistic settings, paving the way for a better understanding of quantum optimization heuristics and the development of improved versions for near-term applications.

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swMATH: A Publication-based Approach to Mathematical Software

By Wolfgang Dalitz, Wolfram Sperber, and Hagen Chrapary

SOFTWARE AND PROGRAMMING

The growing importance of mathematical software in everyday life—in applications such as internet communication, traffic, and artificial intelligence—necessitates advances in software documentation services to raise awareness of existing packages and their usage. Such information helps potential software developers and users make informed choices about packages that could advance their work in modeling, simulation, and analysis. At the same time, software presents novel challenges to information services that require the development of new methods and means of processing.

swMATH[1] provides users with an overview of a broad range of mathematical software and extends documentation services for publications related to such software (see Figure 1). It acts as a counterpart to the established abstracting and reviewing services for mathematical publications and has nearly 30,000 entries, making it one of the most comprehensive documentation services in mathematics.

A Publication-based Approach

swMATH employs a so-called publication-based approach that essentially extracts information about software from existing mathematical literature for documentation purposes (see Figure 2, on page 8). Publications tend to feature two types of software information. On one hand, they contain descriptions of software and provide details about the problem classes, algorithms, and test results. On the other hand, they offer data on software usage and its application areas and findings. swMATH conducts analysis by differentiating between publications that focus on software descriptions (standard publications) and uses (user publications). For example, a search for "integer programming" yields a list of software that includes SCIP, Gurobi, and CPLEX (see Figure 1).

The publication-based approach is successful because a growing number of scientific articles describe or cite mathematical software; for example, swMATH currently has 382,778 software references in 205,487 different articles. Many publications specialize in algorithms and mathematical software, and their analyses yield a great deal of information. As indicated by the aforementioned use of heuristic procedures, the publication-based method is largely automatic. However, accessing the mathematical literature continues to be a major challenge. Large bibliographic databases in mathematics—such as Mathematical Reviews[2] and zbMATH[3]—offer nearly complete and systematic overviews of mathematical publications, beginning in 1868 and 1940 respectively. These databases include reviews, abstracts, keywords, citation lists, and/or mathematical classifications. The data is available in structured form and thus allows for a field-based evaluation.

swMATH adopts heuristic methods—in particular, analysis of characteristic word patterns and art words that are often used as software names—to evaluate zbMATH entries (which will be open access as of 2021). Searching titles and citations is particularly effective. One of swMATH's main features is its ability to link software with the citing literature. Publication metadata in zbMATH entries helps derive a variety of directly and indirectly extracted software metadata.

In the case of directly derived metadata, software descriptions entail a review or abstract of standard publications. Keywords in standard publications characterize the mathematical area, background, and keywords of the referenced user publications. The Mathematics Subject Classification code of standard or user publications uniformly assigns mathematical and application areas. After all, publications that cite software comprise metadata that deliver contextual references and contact persons.

See **swMATH** *on page 8*

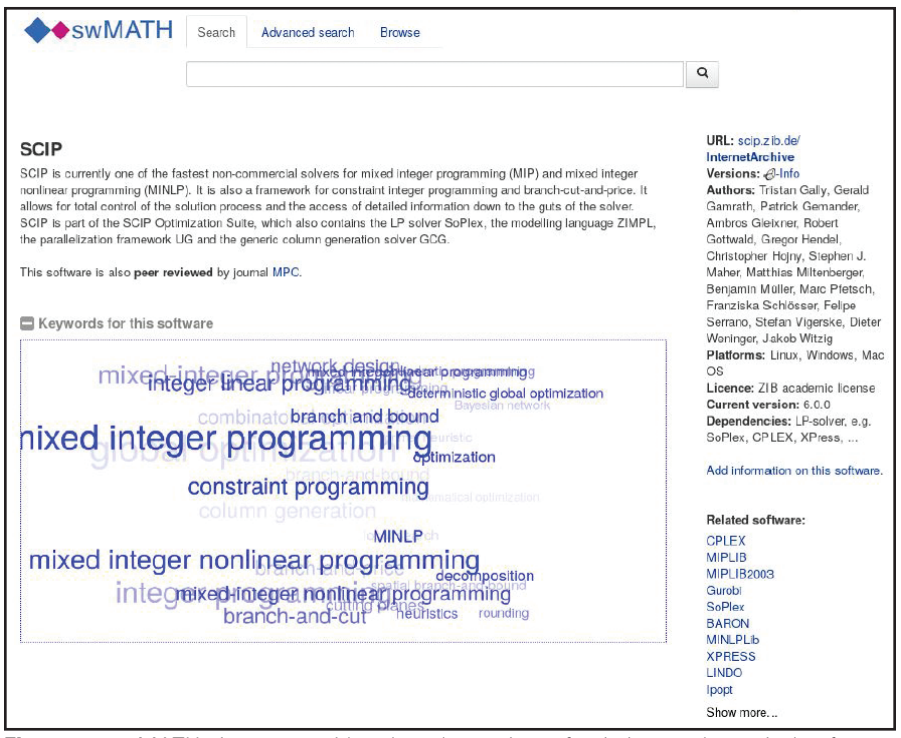

Figure 1. *swMATH aims to provide a broad overview of existing mathematical software. For instance, a search for "integer programming" produces a list of software that includes SCIP, Gurobi, and CPLEX.*

[1] https://swmath.org

[2] https://www.ams.org/mr-database

[3] https://zbmath.org

swMATH

Continued from page 7

For indirectly derived metadata, the relationship between swMATH entries and citations indicates that a software is quoted more than 10 times on average, but the citation numbers are very different. High citation numbers indicate software acceptance and can be considered a metric of quality. Publication data provide information about the software's developmental state. Finally, common citations in zbMATH entries point to similarity or dependency relationships between software artifacts.

Development of Software Documentation Services

Software documentation services must address the needs of both developers and users. Developers often wish to leverage existing software for collaboration or extend its capabilities with further development. And users require software to solve problems of interest, which necessitates the availability of source code, application programming interfaces (APIs), documentation, and user experience information. Users must also have the ability to discover existing software that addresses particular problem classes (integer programming, for example).

A variety of mathematical software information services meet these various needs, including services like GitHub that provide software development environments, especially code development; software archives such as Software Heritage[4] that permanently archive software artifacts; and software documentation services like Wikipedia or software catalogs of user groups.

Accepting Mathematical Software in swMATH

The evaluation of software quality depends on many factors—including correctness, development level, user interface, support, hardware and software dependencies, and licenses—that are also influenced by user perspectives. The swMATH database is limited to entries from distinguished sources that help to ensure software quality:

• **Entries extracted from zbMATH citations:** The publication-based approach ensures that swMATH includes software artifacts cited in the zbMATH database. zbMATH evaluates only peer-reviewed publications, which particularly applies to publication results that are achieved using software. The citation is an indirect indicator of the software's acceptance and subsequent quality. The same applies in principle to entries that result from evaluation of the arXiv repository.

• **Entries obtained from software journals:** Journals specializing in scientific software, like *ACM Transactions on Mathematical Software*[5] or *Mathematical Programming Computation,*[6] also increasingly include verification of reported results.

• **Entries from software repositories:** Software repositories, such as the Comprehensive R Archive Network[7] repository for statistical software, have special requirements for inclusion. These stipulations in turn provide indirect statements about an entry's quality.

Enrichment

One can utilize swMATH entries to link software with related detailed information, including the website, code, or API. Popular software often have their own URLs, though these links are not always permanent. Therefore, swMATH entries link to websites as well as scans of websites that are available in the Internet Archive.

Developer platforms like GitHub are frequently used in the academic sector for distributed creation and further development. These platforms typically provide access to the latest versions of software but do not permanently secure previous software artifacts. Software Heritage has built an archive of software artifacts in recent years that periodically mirror, store, and share all freely available information from key developer platforms. swMATH cooperates with Software Heritage and connects entries to the available software artifacts.

By linking to software websites, the Internet Archive, and Software Heritage, swMATH offers much more than a list of existing mathematical software. Rather, it is a portal for mathematical software that accommodates the needs of various user groups. Nevertheless, the swMATH resource must be further expanded and developed. The publication-based approach means that swMATH entries are subject to delays caused by the publishing process. As a result, other sources—such as the arXiv and mathematical software publications—are included in the evaluation. Data analysis should thus be extended to as many journals as possible. The user interface also enables manual entry of additional information. Furthermore, the portal allows one to embed software in its mathematical context, e.g., by connecting algorithms with possible software implementations. Researchers are currently discussing an extension of the approach that involves linking with algorithms and test data, which seems realistic.

Wolfgang Dalitz is a scientist at Zuse Institute Berlin who works in the field of scientific information systems. He has been involved in building mathematical software libraries since the late 1980s. Wolfram Sperber has been editor of Zentralblatt für Mathematik since 2006. He retired from his position as a senior researcher at FIZ Karlsruhe in 2019. Hagen Chrapary is a software developer at Zentralblatt and Zuse Institute Berlin.

[4] https://www.softwareheritage.org
[5] https://dl.acm.org/journal/toms
[6] http://mpc.zib.de
[7] https://cran.r-project.org

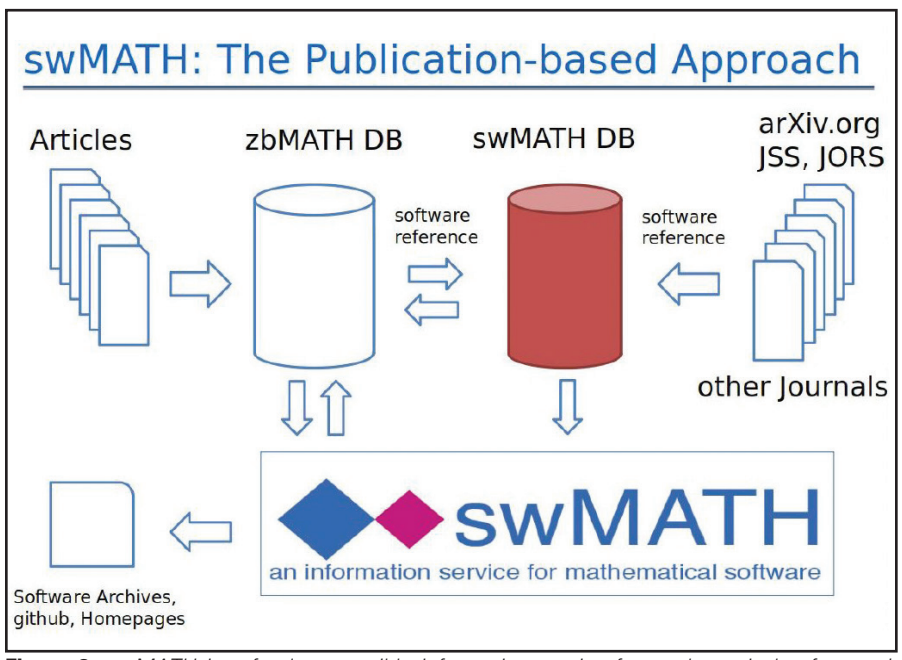

Figure 2. *swMATH is a freely accessible information service for mathematical software. It provides access to an extensive database of information on mathematical software and also includes a systematic linking of software packages with relevant mathematical publications. Figure courtesy of Wolfgang Dalitz.*

From Academia to Major League Baseball: The Journey of a Data Scientist

By Mike Dairyko

CAREERS IN MATHEMATICAL SCIENCES

My love for mathematics blossomed in a linear algebra course during my sophomore year at Pomona College. I felt truly challenged in the subject for the first time, and I enjoyed the sense of accomplishment that came with grasping complex topics. A certain beauty exists within mathematics, inherent in the way that one can prove something given only a few base assumptions and a series of logical statements.

One day, my professor suggested that I apply to the Research Experiences for Undergraduates (REU) program to gain experience in mathematical research. REUs expose undergraduate students to research in their respective disciplines, provide opportunities for networking, and offer a taste of the graduate school experience. REU projects receive funding from the National Science Foundation, which helps support participating undergraduates as they work on research projects at host institutions. During an REU, faculty or researchers from the student's field mentor and teach him/her. I would strongly urge any undergraduate *SIAM News* reader who is interested in graduate school to apply for an REU. Due to encouragement from my professor, I ended up participating in two REU programs during my remaining collegiate summers. The mathematics with which I engaged during the REUs was well beyond the scope of classroom instruction, and both of my REU research groups published our results; I was hooked! My participation in these programs altered my career path and ultimately inspired me to pursue a doctoral degree in applied mathematics at Iowa State University.

In my early years of graduate school, I was convinced that I was going to be a mathematics professor at a small liberal arts college. My vision changed after I took "Introduction to Machine Learning" to complete a cognate course requirement for my degree. Machine learning piqued my interest because it was a combination of mathematics, statistics, and computer science. As the course progressed, I found myself studying machine learning during the time I had set aside for research. Then I discovered data science and knew it was the area in which I wanted to pursue a career.

After earning my Ph.D., I began to look for jobs in the data science community. In my opinion, networking is an essential skill that is worth developing before the job search begins. Throughout my job search, I utilized the professional network that I had built over the course of my undergraduate and graduate years. As a result, I received an invitation to interview for a data science position with the Milwaukee Brewers Baseball Club.

I am currently the Senior Manager of Data Science for the Milwaukee Brewers. I lead the data science portion of the Strategy and Analytics Department for Business Operations and manage another data scientist. My group acts as an internal consultant to support various departments within the Brewers, including Ticket Sales, Stadium Operations, and Marketing. My job scope is broad, but at the core I use machine learning to provide mathematical insights in relation to ticket sales and revenue. I have helped develop models to project game-by-game ticket sales, turnstile, and revenue; likelihood of ticket purchase; marketing impact on ticket sales; and much more. I employ a combination of the programming language Python, database manager SQL, and dashboard tool Tableau to build my models, access and manipulate data, and create visualizations of my outputs.

During the season, one of my main priorities is to produce game-by-game ticket and revenue projections. To do so, my group incorporates historical data—such as team performance, weather, and schedules—into multiple regression-based models and then consolidates the outputs in an easily-digestible format. A large codebase both automates and maintains this process; the codebase is regularly tweaked to ensure that it is agile enough to handle the constant usage and flow of new information. While I take a quantitative approach to creating these projections, the Ticket Sales Department relies on a more qualitative approach with institutional knowledge. A few days before each game, we meet to align the game forecast before distributing it throughout the organization. Most of the time, the delta between the two projections is relatively close. Whenever major discrepancies are present in the numbers, we either find minor bugs in the code or a need to update institutional knowledge. Our projections are most accurate when we utilize both qualitative and quantitative forecasts. These projections are then used for a variety of internal purposes, like concession and usher staffing, season-wide budgeting, and marketing.

See **Major League Baseball** *on page 11*

Mike Dairyko, Senior Manager of Data Science for the Milwaukee Brewers Baseball Club, at Miller Park on opening day in 2019. Photo courtesy of Danny Henken.

Balancing a Knife, Euler's Elastica, and the Mathematical Pendulum

MATHEMATICAL CURIOSITIES
By Mark Levi

While putting dishes in the sink, I tried to balance a knife on the edge of a pot and noticed an interesting effect: the knife balanced, and stably so, if the blade touched the water (see Figure 1). But nothing worked when the pot was empty; the blade was too light.

The Mechanism

Before looking at the photo, one might think that the blade's buoyancy would make the balancing act even more impossible, thus giving the handle further advantage. So what is responsible for the balance and stability? In Figure 1, the blade lifts some water up above the level of the remaining surface; this creates suction that pulls the blade down. The lifted water is then added to the blade's weight, and the equilibrium is automatically stable because the restoring suctional torque is an increasing function of the outward tilt (up to a point). Surface tension also pulls the blade down, but this force is negligible. However, the role of surface tension is indispensable in another way — namely in preventing air from entering the space underneath the blade. To test this role, I added dish soap to the water to see if the decreased tension would cause the knife to tip out. At first nothing happened, but I realized that was because the soap simply dropped to the bottom of the pot. When I mixed the soap with some water and then put it in, the knife tipped out. Soap can decrease water's surface tension by more than half, down from approximately 72 *dyn/cm*.

A Surprisingly Large Force

To estimate the magnitude of the force that is required to break the knife's contact with the water, let us consider a slightly simpler case: a *horizonal* plate of area A touching the water's surface (our knife is slightly tilted, hence the difference). The force required to break contact with the water turns out to be approximately

$$F = 2A\sqrt{\rho g \sigma}, \qquad (1)$$

where ρ is the water's density and σ is the surface tension; I derive this formula at the end. The force is surprisingly large: for the area $A{=}1m^2$, it is about 5 kg, i.e., roughly 10 pounds. In contrast, the surface tension results in the force f approximately proportional to the plate's perimeter P:

$$f \approx \sigma P,$$

which is a much smaller quantity than F for the areas that are the size of our knife.

Euler's Elastica

Consider the shape of the water's surface along the straight edge of the knife in Figure 1, assuming that this edge is also parallel to the surface. Figure 2 depicts the two-dimensional section of this shape, which is governed by the equilibrium condition:

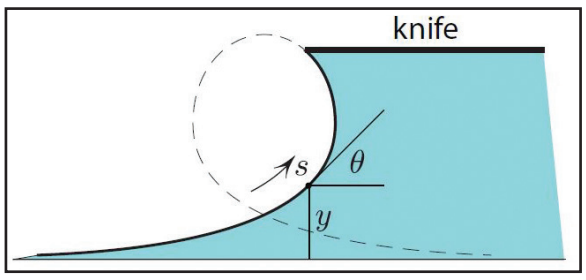

Figure 2. *The shape of the water's surface along the straight edge is an Euler's elastica.*

Curvature κ is caused by the pressure difference p between the two sides of the water's surface[1] *and is inverse proportional to the surface tension* $\kappa{=}p/\sigma$. Since the hydrostatic $p{=}\rho g y$ (the excess of the air pressure over water pressure), we have

$$\kappa = cy, \qquad (2)$$

where $c = \frac{\rho g}{\sigma}$. The exact same equation describes Euler's elastica: equilibrium shapes of elastic rods, except that c can also be negative.

The Pendulum

By differentiating (2) with respect to the arc length s along the curve and recalling that $\kappa = \theta'$ and $y' = \sin\theta$ (here, $' = d/ds$), we get

$$\theta'' = c\sin\theta.$$

This is precisely the equation of the pendulum, with $\theta{=}0$ corresponding to the upside-down (unstable) equilibrium. In other words,

See **Euler's Elastica** *on page 11*

Figure 1. *A knife balances stably on the edge of a full pot if the blade touches the water.*

[1] Actually, one could call it the air's surface with almost equal justification.

Predicting the Shape of Evolutionary Trees

The following is a short excerpt from Phylogeny: Discrete and Random Processes in Evolution by Mike Steel, which was published by SIAM in 2016. This text comes from chapter three, "Tree Shape and Random Discrete Phylogenies," and is modified slightly for clarity.

This excerpt is the first installment of a new SIAM News feature called "From the SIAM Bookshelf," which will periodically spotlight SIAM texts in areas of wide appeal to the greater applied mathematics and computational science community.

FROM THE SIAM BOOKSHELF

The Shape of Evolving Trees

[Extinction has] played a major role in the history of life; after all, most species are extinct.[1] Suppose we sample some subset X of species that are present today (species a-e in Figure 1a) and then consider the minimal tree linking these species. This results in the so-called "reconstructed tree" illustrated in Figure 1b. Let us view this as a rooted phylogenetic X-tree (ignoring the length of the edges). It turns out that under very general assumptions concerning the speciation-extinction process, many models predict an identical and simple discrete probability distribution on $RB(X)$. Moreover, this discrete probability distribution can be easily described and is called the *Yule-Harding* (YH) model (or distribution).

To obtain a binary tree shape under the YH model, we start with a tree shape on two leaves and sequentially attach leaves, attaching a new leaf at each step to one of the leaf edges chosen uniformly at random from the tree constructed so far. For example, the probabilities of generating the fork and caterpillar tree shapes are $\frac{1}{3}$ and $\frac{2}{3}$ respectively, since from the (unique) tree shape on three leaves, we can attach a new leaf to exactly one of the three leaf edges to obtain a fork tree shape, or to any two of these leaf edges to obtain a caterpillar tree shape (see Figure 1c).

Once we have built up a tree with n leaves in this way, we obtain a random tree shape on n leaves and can now label the leaves of this tree shape according to a permutation on $\{1,2,\ldots,n\}$, chosen uniformly at random. This is the YH probability distribution on $RB(n)$.

We now explain how to compute the probability of a YH tree shape and that of any rooted phylogenetic tree with this shape. First, let us grow a tree under the YH process until it has n leaves, and then randomly select one of the two subtrees incident with the root (say, the "left-hand one" since the orientation in the plane plays no role) and let Z_n denote the number of leaves in this tree. Remarkably, Z_n has a completely flat distribution.

Lemma 1. *Z_n has a uniform distribution between 1 and $n-1$, so*

$$\mathbb{P}(Z_n = i) = \frac{1}{n-1}, \text{ for } i = 1,\ldots,n-1.$$

Proof: The random process $Z_1, Z_2, \ldots$ can be exactly described as a special case of a classical process in probability called *Pólya's urn*. This consists of an urn that initially has a blue balls and b red balls. At each step, a ball is sampled uniformly at random and returned to the urn along with another ball of the same color. In our setting, $a=b=1$ and "blue" corresponds to the left-hand subtree and "red" to the right-hand subtree in the YH tree. At each step, the uniform process of leaf attachment ensures that Z_n has exactly the same probability distribution as the number of blue balls in the urn after $n-2$ steps. It is well known, and easily shown by induction, that in Pólya's urn with $a=b=1$, the proportion of blue balls has a uniform distribution.

Lemma 1 provides the key to computing the YH probability of a tree.

Proposition 1. *For any particular tree $T \in RB(n)$, the probability $\mathbb{P}_{\text{YH}}(T)$ of generating T under the YH model is given by*

$$\mathbb{P}_{\text{YH}}(T) = \frac{2^{n-1}}{n! \prod_{v \in \mathring{V}(T)} \lambda_v},$$

where $\mathring{V}(T)$ is the set of interior vertices of T and λ_v is number of leaves of T that are descendants of v, minus 1.

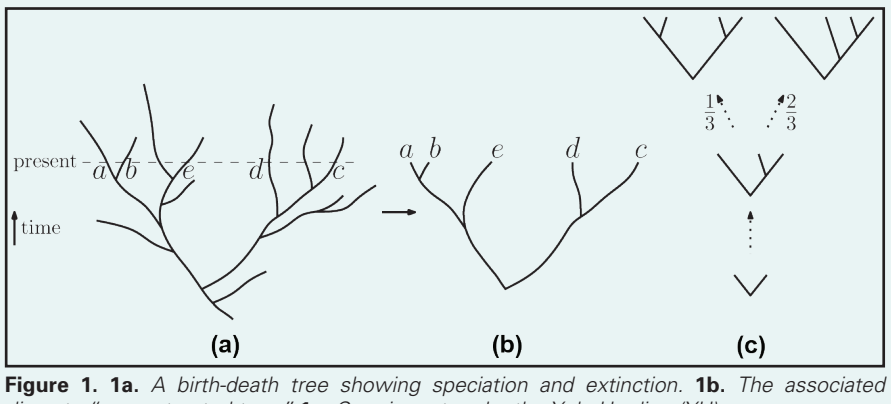

Figure 1. 1a. *A birth-death tree showing speciation and extinction.* **1b.** *The associated discrete "reconstructed tree."* **1c.** *Growing a tree by the Yule-Harding (YH) process.*

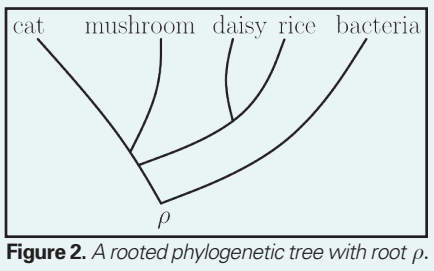

Figure 2. *A rooted phylogenetic tree with root ρ.*

Proof: Suppose that the two maximal subtrees T_1 and T_2 of T are of size k and $n-k$, where we may assume that $2k \le n$. By Lemma 1, the probability of such a size distribution is $2/(n-1)$ if $2k < n$ and $1/(n-1)$ if $2k = n$. Conditional on this division, the number of ways to select leaf sets for T_1 and T_2 that partition $[n]$ is $\binom{n}{k}$ when $2k < n$ and $\frac{1}{2}\binom{n}{k}$ when $2k = n$ (the the factor of $\frac{1}{2}$ recognizes that the order of T_1 and T_2 is interchangeable in T when they have the same number of leaves). By the Markovian nature of the YH process, each of these two subtrees also follows the YH distribution. This leads to the recursion

$$\mathbb{P}_{\text{YH}}(T) = \frac{2}{n-1}\binom{n}{k}^{-1} \mathbb{P}_{\text{YH}}(T_1)\mathbb{P}_{\text{YH}}(T_2),$$

from which Proposition 1 now follows by induction.

To illustrate Proposition 1, consider the tree in Figure 2. Then we have $\mathbb{P}_{\text{YH}}(T) = \frac{2^4}{5! \times 4 \times 3 \times 1^2} = \frac{1}{90}$, while the tree in Figure 1b gives $\mathbb{P}_{\text{YH}}(T) = \frac{1}{60}$.

Exercise: Find a general formula for the probability that a random tree $\mathcal{T}$ in $RB(n)$ generated by the YH model has the shape of a rooted caterpillar tree. What is the probability that $\mathcal{T} = T$ for a particular caterpillar tree $T \in RB(n)$?

Curiously, a quite different process that arises in population genetics, and which proceeds backward in time (rather than forward, as in Figure 1c), also leads to the YH distribution when we ignore the length of the edges and the associated ranking of interior vertices. This is the celebrated *coalescent* process most usually associated with Sir John Kingman and developed in the early 1980s. As a discrete process, the coalescent starts with the set X and selects uniformly at random a pair of elements to join (these form the "cherry" of the tree that is closest to the leaves). These two leaves are then regarded as a single element in a set of size $|X|-1$, and the process is repeated. This discrete coalescent process generates a ranked binary phylogeny, which is often referred to as a *labeled history*. This consists of a pair (T, r), where $T \in RB(X)$ and r is a *ranking* of the interior vertices of T — that is, a bijective function $r : \mathring{V}(T) \to \{-1, -2, \ldots, -(n-1)\}$ with the property that if u is a descendant of v, then $r(u) > r(v)$ (thus the root is the vertex assigned an r value of $-(n-1)$). The function r describes the order in which the coalescent events occur, so the first cherry to form in the process has rank -1, for instance.

Enjoy this passage? Visit the SIAM bookstore at ***https://my.siam.org/Store*** *to learn more about Phylogeny: Discrete and Random Processes in Evolution and browse other SIAM titles.*

Mike Steel is director of the Biomathematics Research Centre at the University of Canterbury in New Zealand. He works on mathematical modelling of processes in evolution and related areas.

[1] It is estimated that current plant and animal diversity preserves at most one to two percent of the species that have existed over the past 600 million years.

Major League Baseball

Continued from page 9

A typical day at Miller Park, home of the Milwaukee Brewers, tends to involve a balance of individual and group work. I usually begin with a team meeting to provide status updates on various projects and offer assistance for any problems that arise within the group. I then spend most of my time developing SQL queries and Python scripts to assist with larger projects or answer various questions for upper management. I also handle administrative tasks that aid in the distribution of various model outputs to individuals within the organization. Sometimes I meet with personnel from other departments to discuss and interpret model projections. And whenever there is a game during work hours, I take a break and watch an inning or two in the ballpark!

Mathematicians are ultimately trained to develop problem-solving skills and apply them with persistence and creativity. For example, they will likely face many failed attempts when completing a problem set or conducting research. Carefully reviewing the work—and perhaps redoing it a different way or approaching the issue from another angle—eventually leads to success. I liken my position's level of difficulty to that of conducting research for my dissertation. With that said, I do not apply the same high-level proof techniques from graduate school to my current work. However, I do use the problem-solving strategies, persistence, and creativity that I have honed throughout my mathematical journey every single day.

Although my path to becoming a data scientist was not necessarily linear, I have learned a great deal on the way and can share a few recommendations for those interested in a career in data science. I would encourage students to become comfortable with navigating a programming language such as R or Python. These languages are extremely powerful and indispensable for advanced modeling. Note that a lot of free online content is available to assist with broadening programing skills. Briefly stepping outside of mathematics and establishing computer science and statistics expertise is also useful. In retrospect, doing so would have greatly benefited me. Finally, participating in conferences with data science content is an excellent way to gain exposure to more advanced topics in the field and build a network within the community.

Mike Dairyko is currently the Senior Manager of Data Science for the Milwaukee Brewers Baseball Club. He also is an adjunct professor in the Lubar School of Business at the University of Wisconsin-Milwaukee.

Euler's Elastica

Continued from page 10

if we travel along the curve in Figure 2 (on page 10) with unit speed, the tangent's direction swings exactly as if it were a pendulum (with gravity pointing to the left in Figure 2). The curve in Figure 2 satisfies $\theta \to 0$ as $s \to -\infty$ and $\theta \to 2\pi$ as $s \to +\infty$. This corresponds to heteroclinic solution of the pendulum equation, with the pendulum approaching the unstable equilibrium in both future and past.

Derivation of (1)

The force F is the weight of the lifted water of volume $\approx AH$, where H is the maximal possible height, so that

$$F \approx \rho g A H. \tag{3}$$

We must find the maximal possible H for which the surface tension can still keep the air from under the plate.

According to Figure 3, the equilibrium condition is

$$2\sigma L = p_{\text{average}} \cdot HL. \tag{4}$$

After simple algebra, substituting $p_{\text{average}} = \frac{1}{2}\rho g H$ into (4) yields

$$H = \sqrt{\frac{4\sigma}{\rho g}}.$$

Substituting this value into (3) gives the lifting force (1). This is the theoretical maximum; the true value may be less because the angle θ near the top need not be π, as it is in Figure 3.

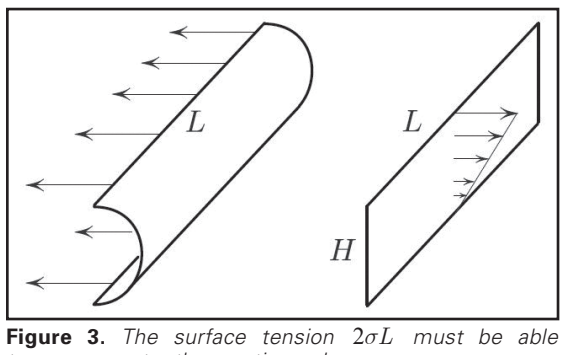

Figure 3. *The surface tension $2\sigma L$ must be able to compensate the suction whose average pressure between $y=0$ and $y=H$ is $p_{\text{average}} = \frac{1}{2}\rho g H$, thus producing the force $p_{\text{average}} HL$.*

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.

Computational Topology in Geometric Design: Manifolds to Molecules

By Kirk Gardner, Kirk E. Jordan, Alex Harrison, James L. McDonagh, Breanndán Ó Conchúir, Thomas J. Peters, and Donald R. Sheehy

While computational topology enjoys considerable contemporary prominence, it is certainly not an overnight success story. The field's prosperity relies heavily upon classical foundations from general, geometric, algebraic, and low-dimensional topology. Here we explore applications that range from manifolds for airfoils to molecules for pharmaceuticals.

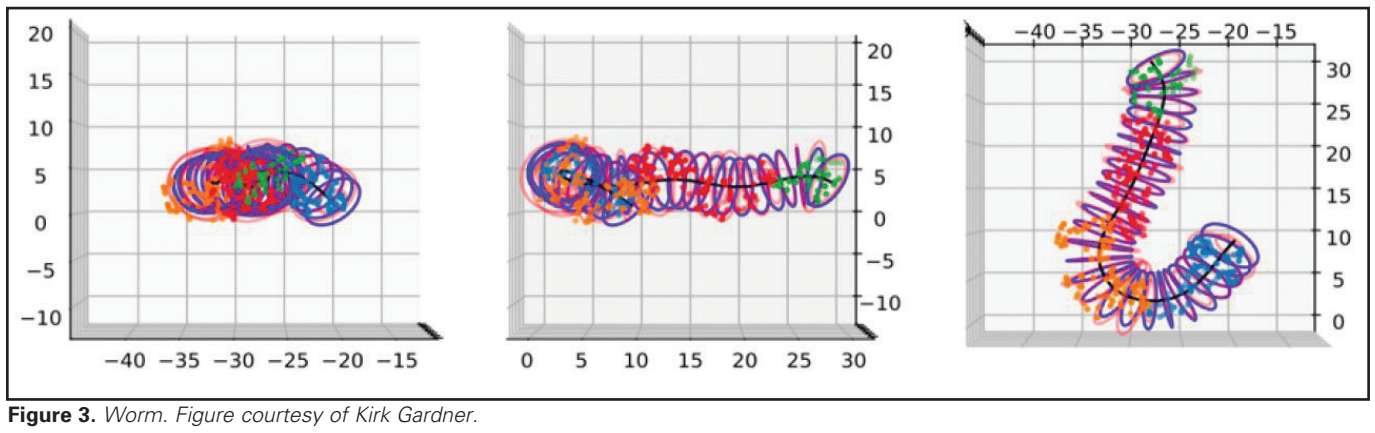

Figure 3. *Worm. Figure courtesy of Kirk Gardner.*

Introduction, History, and Manifolds

The first usage of the term *computational topology* likely occurred within a 1983 doctoral dissertation on computer aided geometric design (CAGD) [10]. Two decades later, pioneers in topological data analysis (TDA) greatly popularized the term [5, 7]. This article emphasizes geometric topology for analysis of point clouds, suggesting promise for the integration of CAGD and TDA techniques under the broad abstractions of applied topology [8].

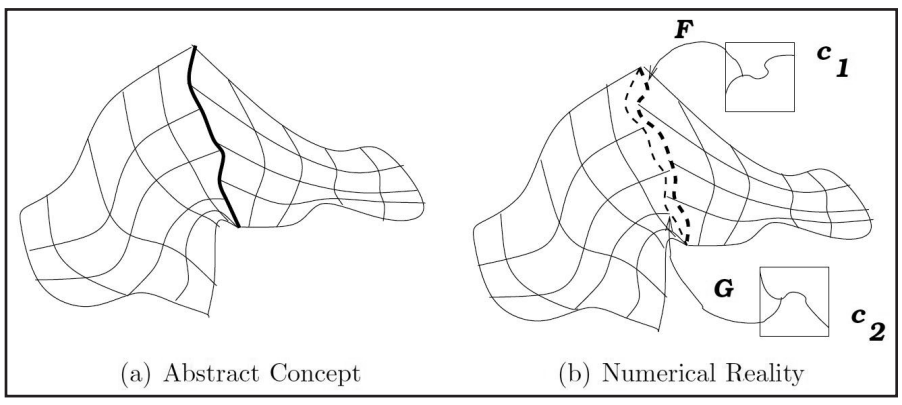

Figure 1. *Surface intersection for boundary. Figure courtesy of Thomas Peters.*

Within geometric design, boundary surfaces of solids frequently form from the intersection of two surfaces, which then join along this intersection (see Figure 1a). Practical complications arise, as numerical computations yield deviations from this abstract theory [9]. Researchers often assume that the intersected surfaces are manifolds, so algorithmic detection of self-intersections is an important focus [2]. Figure 1b depicts numerical errors between two manifolds that are joined along their intersection curves [4]. We model the surfaces as splines and compute two pre-images of the intersection curve (one in each surface's parametric domain); these actions lead to the indicated numerical differences since the curves are instantiated on each surface. Considerations in aeronautical design and engineering for modeling fuselages and wings inspired Figure 1.

CAGD's success revolutionized engineering design and manufacturing. Boundary representation (B-rep) models became a dominant approach to topological representations [9, 11], and general topology, combinatorial topology, low-dimensional topology, and knot theory for isotopic equivalence provided supporting ideas [1]. Researchers focused heavily on the adaptation of "pure topology" concepts to finite precision data [9, 11].

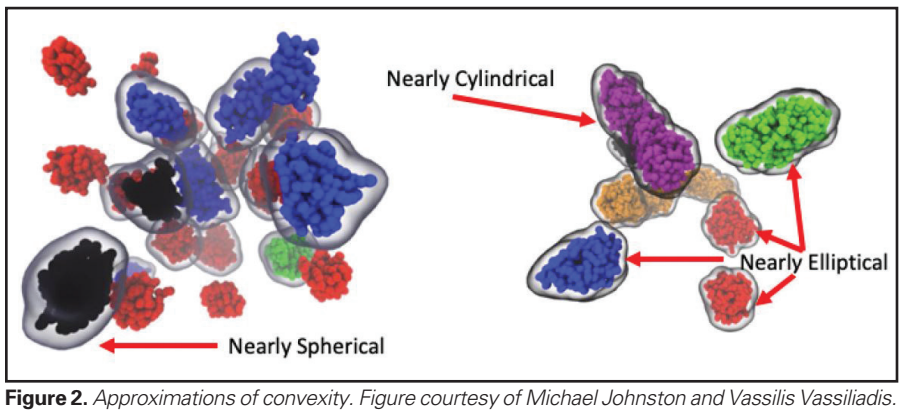

Figure 2. *Approximations of convexity. Figure courtesy of Michael Johnston and Vassilis Vassiliadis.*

Data for Molecules

Here we apply geometric topology to data pertaining to molecules' point clouds, which we generated from supercomputer simulations of dissipative particle dynamics. This adaptation of computational topology from CAGD to computational chemistry and chemical engineering extends the rich history of topological modeling in chemistry [12]. The corresponding examples are micelles, which are optimized for industrial applications of controlled drug release, household cleaning products, and friction modifiers in vehicle engines [6]. The annotations of Figure 2 distinguish micelles that are "approximately convex" from "worms," which are the focus of current research.

While convexity is solely a geometric property, extraction of the topological boundary accelerated the algorithmic identifications. This was based upon a heuristic that any point having six or more adjacent points was an interior point (all pairwise Euclidean distances were pre-computed, with unit distance as the upper bound for adjacency since no exterior points existed). The approach typically reduced the data by an order of magnitude, whereas the resulting image is representative of one video frame. This data reduction permitted algorithmic shape identification to run synchronously with the simulation.

In its simplest form, a worm is like a twisted garden hose (see Figure 3). A central axis to approximate the length is of particular interest for chemical analysis. In simplified worms, one can extract such a skeleton with adaptations of the medial axis (MA), which is topologically unstable. Empirical algorithmic refinements attained topological stability for the given data. Piecewise linear approximations to the MA were especially appropriate, as is also often true in CAGD.

Figure 4 depicts a worm's additional topological complexities. This worm is a non-convex, simply connected shape, but its skeleton is not homeomorphic to a line segment. Chemists visually identified the thin bridging (near the center of Figure 4) as structurally important.

Researchers developed special purpose algorithms to create responsive branched skeletons. They first computed discrete Laplacians and the Fiedler gap to generate clusters in point clouds [3], then connected the centroids to form an initial piecewise linear (PL) approximation of the skeleton. Further refinements extended line segments to the extreme points of the topological boundaries. Next, scientists calculated the skeleton's total length as a sum of the lengths of the segments in the PL skeleton, and estimated an average value of the cross-sectional radius around the skeleton. They used these two parameters for computational chemical analyses [6], which strongly corroborated postulated theories about micelles.

Concluding Thoughts

Here we share some of topology's rich interaction with geometric modeling and design. A similarly robust synergy is simultaneously occurring between topology and data analysis. The former relies more heavily on geometric and differential topology, while the latter depends on algebraic topology. As big data is also a prominent component of design, we invite readers to consider synergy between these two facets of computational topology, as expressed here and in the January/February 2020 issue of *SIAM News*.[1]

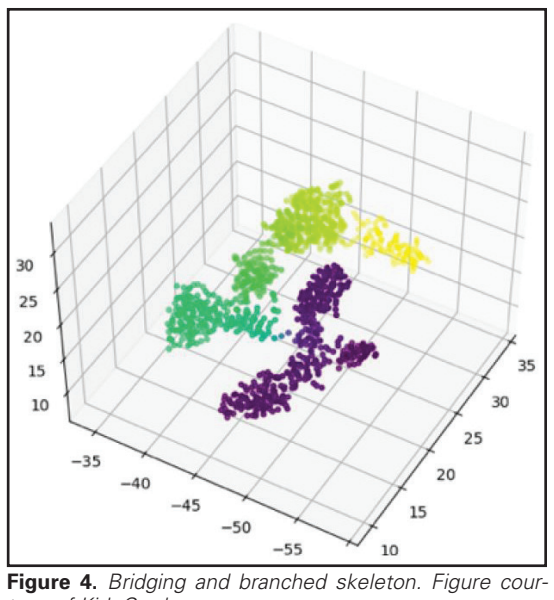

Figure 4. *Bridging and branched skeleton. Figure courtesy of Kirk Gardner.*

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