Deep Learning for COVID-19 Diagnosis

By Keegan Lensink, William Parker, and Eldad Haber

O
er the last several months, the severe acute respiratory syndrome coronavi-
sus 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 syn-
drome—the most common presentation
associated with morbidity and mortality is
the presence of opacities and consolid-
ation 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 opaci-
fication is visible on computed tomography
(CT) scans. Due to their increased densi-
ties, these areas appear as partially opaque
regions with increased attenuation, which
are known as a ground-glass opacity (GGO).
Consolidation occurs when the accumula-
ton of fluid progresses to an opaque region
on CT scans (see Figure 1).

As COVID-19 spreads, healthcare cen-
ters around the world are becoming over-
whelmed 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 ventila-
tion, both of which have limited availabil-
ity. Rapid screening is crucial in diagnosing
COVID-19 and slowing its spread, and
effective tools are essential for prognostica-
tion 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 environ-
ments 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 diag-
nostic process, including follow-up assess-
ment 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
can enable highly sensitive diagnosis [1].

In addition to providing complimen-
	ry 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 percent-
age 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
scans enables high sensitivity and specificity.

Modeling Population Recovery
Following an Environmental Disturbance

By Azmy S. Ackleh and Amy Veprauskas

What do populations of invasive and
damaged 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 communi-

ties [7]. This means that their presence and
densities help shape community composi-
tion. Because they are granivores, kanga-
roo rats significantly impact annual plants
that serve as a resource base [4]. However,
these communities are subject to vari-

dious disturbances—including habitat frag-
mentation, 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 disrup-
tions [5]. The 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 bull-
frog tadpoles’ voracious appetites may dra-

matically 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 habi-
tats, changing ecosystem structure and even
causiNG local extinctions among native spe-
cies. Control methods for American bull-

frog tadpoles typically focus on the removal
of tadpoles or adults from the population.

What similarities exist between these
two scenarios? In addition to both popula-
tions substantially impacting overall com-

munity structure, these situations have two
common components. Both cases involve
the idea of a disturbance—such as habi-
tat 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 expe-

rience natural and anthropogenic distur-

bances—like hurricanes, fires, and chemi-

cal and noise pollution—that negatively
affect 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 conser-

vation approaches, or aid in the establish-
ment 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
mentioned approach for bullfrog regula-
tion might be an ineffective means of
population control, and in some cases actu-
ally result in increased population sizes.
Instead, removal of metamorphs in the fall

Figure 1. Visualization of an axial slice of a computed tomography (CT) scan, cropped to the left lung. (a) Pulmonary opacification present in a patient with COVID-19. (b) 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.

Figure 1. Recovery time’s sensitivity to properties of the disturbance. (a) Recovery time’s sensitivity to changes in survival reduction $\epsilon$, assuming a 10-year duration of impact. (b) Duration of impact $T_0$, assuming a five percent reduction in survival. Figures adapted from [1].
5 The Mathematics of Mass Testing for COVID-19

David Donoho, Mahsa Lotfi, and Bamtezar Markazi explore an emergent research front in which mathematical and statistical models can enable a rapid expansion of COVID-19 testing capabilities worldwide. Donoho surveyed these findings and presented several related research projects during a virtual invited presentation at the 2020 SIAM Conference on Mathematics of Data Science.

6 Chaos (and Dynamos) for All!

The field of dynamical systems is ever-changing, and mathematicians continue to enhance concepts that inspire a greater understanding of order and disorder. Lora Billings reviews David Feldman’s Chaos and Dynamical Systems, a new book that introduces the field and addresses models of both discrete and continuous dynamical systems, ultimately engaging readers at a variety of levels.

7 swMATH: A Publication-based Approach to Mathematical Software

The growing importance of mathematical software in everyday life necessitates advanced approaches to software documentation. Wolfgang Dalitz, Wolfram Sperber, and Hagen Cherpawy describe swMATH, which employs a publication-based approach. This innovative information service provides users with an overview of a broad range of mathematical software and extends documentation services for publications related to such software.

8 From Academia to Major League Baseball: The Journey of a Distinguished Mathematician

Mike Dariyko, a data scientist for the Milwaukee Brewers Baseball Club, details the career trajectory and educational experiences that led him to his role. Dariyko discusses his use of data science and machine learning to provide mathematical insights and calculated projections in relation to revenue, ticket sales, and player market endeavors for the Brewers.

9 Obituary: Bernard J. Matkowsky

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

On June 11, 2020, our friend and colleague Bernard 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 in 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 the General Electric Polytechnic Institute before eventually moving to Northwestern, where he remained for the rest of his career.

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 topics. Bernie’s colleagues and peers regularly cite his recognition of the importance of combustion 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 in the world. Outside of his department at Northwestern, Bernie remained an active member of SIAM. In 2010, he was elected to the SIAM Journal on Applied Mathematics for 18 years (1977-1994), which included a stint as associate managing editor (2002-2004). He also acted as vice chair of the SIAM Activity Group on Dynamical Systems (1988-1990). In 2017, Bernie and his wife, Karen, were recipients of the John von Neumann Prize and delivered the associated prize lecture at the 2017 SIAM Annual Meeting.

Bernie was an outstanding advisor, mentor, and friend to his students, preparing them for successful careers in applied mathematics and science. Bernie is survived by his wife, Karen, his daughter, Daniel, and six grandchildren. Those whose lives he touched will never forget him for his support, energy, and dedication to 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 these individuals interacted extensively with Bernard Matkowsky for many years.

7.8mMATH.png

Photo courtesy of Alvin Bayliss.

LETTER TO THE EDITOR

To the Editor:

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 wait? In one of his last contributions to the mathematics community, Bernie stated what we must do to gain the respect and privileges of faculty in MSS departments; in return, MSS departments must support our research and privileges of faculty in MSS departments; in return, MSS departments must support the research and privileges of faculty in MSS departments.

Bernie was an outstanding advisor, mentor, and friend to his students, preparing them for successful careers in applied mathematics and science. Bernie is survived by his wife, Karen, his daughter, Daniel, and six grandchildren. Those whose lives he touched will never forget him for his support, energy, and dedication to Northwestern and throughout the country, will remain a lasting legacy.

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Solving Combinatorial Optimization Problems on Quantum Computers

By Yuri Alexeev, Jeffrey Larson, Sven Leffler, 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 approximate 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 leverage the best-known approximation ratio for a specific maximum satisfiability problem (Max-3SAT), which has come to be regarded as a useful and well-developed classical algorithm. While QAOA has yet to theoretically improve upon the best classical algorithm for this class, it continues to attract interest within the quantum computing and optimization communities.

Population Recovery

Continued from page 1

may be more effective [8]. And while live-

stock grazing is generally believed to nega-

tively impact some species’ environments, research has shown that livestock promote kangaroo rat recovery if it reduces vegetation cover [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, models can provide useful insights—even when limited data is available—and help generate hypotheses that can be tested in the field. 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 con-

sideration, a population’s recovery may take many forms. If we wish to mathemat-

ically model recovery, we must define the way in which a species’ size changes over time. To do this, we describe a population using a matrix model that allows us to distinguish between individu-

als in different developmental stages. Consider a female population that is divided into m stages. Denote the den-

sities of these stages at time t with n(t); QAOA is one of few algorithms that can reliably run on near-quantum devices. QAOA and its generalization—the quantum alternating operator ansatz [4]—can also tackle a wide class of combinatorial opti-

mization problems that are computationally difficult and intractable in classical models. To dissect 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:

\[ \min_{y \in \{0,1\}^n} f(y) = \sum_{y \in \{0,1\}^n} w(y) \mathbb{1}(y), \]

where the first formulation is an equiv-

alent representation of \( y \) and \( L(y) \) is the indicator function that takes the value 1 if \( y = 0 \) or 0 otherwise. Notice that construction of such an indicator polynomial is sim-

ple, might require 2^n terms in the sum.

This technique can convert the objective function \( \mathcal{f} \) which acts on the boolean hypercube into an operator \( f \) that acts on the continuous hypercube [3, 4]. One can thus endow it with a non-linear structure that allows for more effective quantum search algorithms.

QAOA is one of few algorithms that can tackle a wide class of combinatorial optimization problems that are computationally difficult and intractable in classical models. To dissect 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:

\[ \min_{y \in \{0,1\}^n} f(y) = \sum_{y \in \{0,1\}^n} w(y) \mathbb{1}(y), \]

where the \( \mathbb{1} \) operator denotes the Kronecker product and the vec operator converts a matrix into a column vector by stacking the matrix’s columns. In a simi-

lar 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 (3) and (4), we present an application that inves-

tigates the recovery of sperm whales, which are impacted by a variety of disturbances that impact oil spills and noise pollution. We use a discrete-time stage-structured model to examine a sperm whale popula-

tion [3]. In Figure 1 (on page 1), we present the recovery time’s sensitivity to changes in a sperm whale population with respect to changes in the magnitude of impact \( i \) and duration of impact \( T \). These graphs highlight that the recovery time is more sensitive to changes in \( i \) than in \( T \). For instance, consider the effect of a 10% increase in \( i \) versus a 10% decrease in \( T \). If \( i \) increases, we see a slightly greater percentage increase in recovery time than when \( T \) decreases.

How Sensitive are Recovery Predictions?

Sensitivity analysis measures the way in which small perturbations in a model param-

eter affect model output. When examining a population’s recovery, the recovery time’s sensitivity to an input can help identify the most effective management or control strategy. One can calculate sensitivity in its simplest form by taking a derivative. Using (3) to model recovery, we can find the recovery time’s sensitivity by implicitly diff-

erentiating this equation. For instance, the sensitivity of the recovery time with respect to the magnitude of impact is given by

\[ \frac{d{T_*}}{di} = \frac{\partial{T_*}}{\partial{L}} \frac{\partial{L}}{\partial{i}} \frac{\partial{i}}{\partial{L}} \frac{\partial{L}}{\partial{w}} \frac{\partial{w}}{\partial{T_*}}. \]

Sensitivity analysis of the recovery time for a population under the impact of an envi-


munity delays recovery of dominant com-


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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 WL 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—such as the segmentation of objects on a street, wherein a nonexpert can easily identify the classes—are utilized daily for the diagnosis of COVID-19 patients. Similar to other medical imaging, CT scans provide insight into an infection’s severity by identifying numerous patterns of opacification. However, CT scans provide insight into an infection’s severity by identifying numerous patterns of opacification (see Figure 2). 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 CT image’s clinical implication requires a 3D understanding of structures. Previous researchers have employed 3D CNNs, mainly for video. However, these methods are based on deep learning-based methods in vision. These methods are based on a simple model:

\[ Y_j = f(Y_{j-1}, \theta), \quad j = 1, \ldots, n, \]

where \( Y_j \) specifies hidden layers, \( Y \) is the original 3D image, and the function \( f \) (which depends on the parameters \( \theta \)) is typically composed of convolutions and a non-linear activation function. One of the most successful architectures in recent years employed a function of the form \( f(Y_{j-1}, \theta) = (Y_{j-1} + \theta \cdot Y_j) \). This architecture, called a residual method, is linked to the discretization of the ordinary differential equation (ODE) [4].

\[ Y = G(Y_0, \theta), \]

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 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 the classes. 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 Canada. Volunteer physicians in Vancouver annotated this data, obtaining a large and diverse dataset for training, validating, and testing. Although we initially imagined working with fairly standard networks and optimizations for segmentation, we quickly encountered two major problems. The first problem is the variability between physicians in terms of the “correct” segmentation. Our images are very different from classic 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).

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, a method 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 one to train deep networks on high-resolution 3D images. They are based on the leapfrog discretization of the second-order ODE.

\[ Y = G(Y_0, \theta), \]

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.

This work is based on Eldad Haber’s minisymposium presentation at the 2020 SIAM Conference on Mathematics of Data Science (MD20), which occurred virtually in May and June. Haber’s presentation is available on SIAM’s YouTube channel.2

The figures in this article were generated by the authors.

References


Kregan Lensiuk is a graduate student at the University of British Columbia and a research scientist at Xtract AI. William Parker is a medical doctor and radiologist resident at the University of British Columbia and founder of SapienML. Eldad Haber is a scientific and Natural Sciences and Engineering Research Council of Canada (NSERC) industrial research chair at the University of British Columbia.

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

2 https://www.youtube.com/watch?v=GCLyjy44bKk

Pattern Description Class Number Group Number

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

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

Figure 3. Variability between 12 physicians who segmented the same image slices.
The Mathematics of Mass Testing for COVID-19
By David Donoho, Mahsa Lotfi, and Batu Ozturkler

Obel 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 emerge from its current paralysis. Romer, who previously served as Chief Economist of the World Bank, proposes a confidence-inspiring path out of the shutdown based on dramatically expanding 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. Romer’s solutions are related to 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 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 his talk at the virtual 2020 SIAM Conference on Mathematics of Data Science (MDS20), 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. Mathematicians 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 papers were flooding in daily. Submissions covered everything from individual case reports and documentation of care protocols to fully-developed articles about therapeutic interventions and new journals. Contributors included doctors sharing patient data, medical teams conducting clinical trials, public health officials analyzing national databases, 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 highlighted 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 [3]. 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 can determine whether anyone among a group of 64 patients has the disease.

One common principle is to pack samples 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 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 x of N viral load measurements will be sparse (mostly zeros) because the majority of people are not infected. Mathematically, the problem thus seeks to find most efficiently, with fewest possible round-trip test kits and the least possible wall-clock time delay—determine which entries are nonzero in a large, sparse vector of viral counts.

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 tests into a 2 x 1 vector y. The tested viral loads y are related to the original viral loads via a matrix multiplication y = Ax, where A is a 2 by N binary matrix that indicates which patients’ samples contribute to which test pools. Now the problem involves inferring the sparse vector x from (noisy, partial, binary, and linear) information about y. Researchers sometimes employ multiple rounds of measurements: y = Ax_1 + … + Ar y = A r, R = 1, …, r. With round r+1 pooling matrix A_r dependent on the last round’s test results y_1, …, y_r, one can then infer x from y = [y_1, …, y_r], once again obeying y = Ax — now with block matrix A=[A_1, …, A_r]. Scientists could model A with appropriate use of randomness or delicate constructions that involve special graph structures, sparse matrix patterns, or even information-theoretic codes.

Eventually, one deciphers the test results y = Ax_1 + … + Ar y = A r, R = 1, …, r. 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, x, y) and assumed sparsity of 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 [1, 2] and another employed compressed sensing [4]. Both techniques propose one-round-only methods that show—in part—that they can successfully infer the disease status of N patients from T tests at low levels of population prevalence, where

N \approx 10^T \quad \text{(1)}

When successful, this marks a tenfold expansion in the number of patients whose disease status 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, proceeding 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 mathematical-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 available on SIAM’s YouTube channel.

References

David Donoho is a professor of statistics and the Anne and T. Robert M. Bass Professor of Humanities and Sciences at Stanford University. He has delivered SIAM’s John von Neumann Lecture and is a recipient of the AMS-SIAM Norbert Wiener Prize in Applied Mathematics. Mahsa Lotfi is a postdoctoral researcher in the Department of Statistics at Stanford University. She received her Ph.D. in electrical engineering and signal processing from the University of Texas at Dallas. Batu Ozturkler is a first-year Ph.D. student in the Department of Electrical Engineering at Stanford University.
Quantum Computers

Continued from page 3

We use a classical optimizer to vary the free parameters $\beta, \gamma$ and bring $\langle x \mid \langle x \rangle \rangle$ as close as possible to the basic vector $|e\rangle$ that encodes the result of a classical optimization. This is the original problem’s solution. We have thus replaced the combinatorial optimization over $e$ with a nonconvex optimization over $\beta, \gamma$. 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 $\langle x \mid \langle x \rangle \rangle$ using fidelity $(\langle e \rangle, |e\rangle)^2$. If $\langle e \mid \langle x \rangle \rangle = |e\rangle$ the measurement result will be $|e\rangle$ with probability 1. Realistically, one can only efficiently sample from the output of QAOA under reasonable complexity theory with a measurement that is exact in one step ($p=1$). However, the fact that QAOA is classically hard to simulate does not speak to its potential for solving optimization problems. The second limiting consideration is the performance on problems of realistic size. The dearth of methods to reliably and efficiently solve the parameter optimization problem limits the realization of its potential. Any given problem and depth have a priori knowledge of the parameter values $\beta$ and $\gamma$ that are close to the optimal values that maximize $f$. We must therefore search for these values, often with classical numerical optimization routines. While the optimization appears to be simple in higher depths ($p=1$), QAOA’s most promising regime is shallow (small constant depth) because it can run on near-term hardware. For small depth, the objective over $\beta$ and $\gamma$ is often nonconvex and therefore is not always sufficient to get local optima. Figure 1 (on page 3) is an example objective landscape in the $p=1$ case. QAOA’s performance on a real problem depends critically on the quality of the parameters $\beta$ and $\gamma$. However, a single local optimization run is the classical optimization toward QAOA packages, even though the objective has many suboptimal local optima. One can gain considerable improvement via multi-start optimization strategies [9] or machine learning approaches [6], yet these techniques also struggle when $p$ is a moderate size. The performance of the classical optimization routine for identifying parameters within QAOA is largely an open question. However, one possible consideration is the required large number of qubits and fast, high-fidelity gates to execute QAOA circuits with $p \geq 1$. Classical algorithms can achieve excellent approximation ratios in minutes—no if seconds—for most practically interesting binary optimization problems with less than a few hundred variables. Therefore, until quantum hardware with hundreds of qubits is accessed, 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 few years. Hardware size is growing steadily, but simply increasing the qubit count is not enough. As QAOA gate count grows linearly with the problem description and depth $p$, they quickly surpass classical hardware’s capabilities. For example, QAOA requires execution of $d \cdot n \cdot p \cdot 2^p$ gates for MAXCUT on a $d$-regular graph on $n$ nodes with depth $p$ (assuming full connectivity and using phase flip as the ‘controlled NOT’ as the native 2-qubit gate). This in turn necessitates the execution of $2^p$ gates, which for $2^p \approx 10^2$ gates is exponential and ‘controlled NOT’ as the native 2-qubit gates). 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swMATH: A Publication-based Approach to Mathematical Software

By Wolfgang Dalitz, Wolfram Sperber, and Hagen Chrapary

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 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 and zbMATH—offer nearly complete and systematic overviews of mathematical publications, beginning in 1868 and 1940 respectively. These databases include reviews, abstracts, keywords, citation lists, and mathematical classifications. The data is available in structured form and thus allows for a field-based evaluation.

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 key-words 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.

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.

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.
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 that permanent 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 software implementations. Researchers are currently discussing an extension of the approach that involves linking with algorithms and test data, which seems realistic.

• Entries obtained from software journals: Journals specializing in scientific software, like ACM Transactions on Mathematical Software5 or Mathematical Programming Computation,6 also increasingly include verification of reported results.

• Entries from software repositories: Software repositories, such as the Comprehensive R Archive Network7 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 mirrors, 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 2008. 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.

5 https://www.softwareheritage.org
6 https://mpc.zib.de
7 https://cran.r-project.org

swMATH: The Publication-based Approach

Software Archives, GitHub, Internet Archive

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.

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

By Mike Dairyko

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 grappling 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 them. I would strongly urge any undergraduate student to participate 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, stubulite, 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 sales 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.

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

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 horizontal 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

$$F = 2A \sqrt{\rho g},$$

(1)

where $\rho$ is the water’s density and $\sigma$ is the surface tension; I derive this formula at the end. The force is surprisingly large: for the area $A = 1 \text{ cm}^2$, 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 $P$:

$$f \propto P,$$

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:

$$\kappa \sigma = \rho g y,$$

(2)

where $\kappa$ is the intrinsic curvature of the curve along the surface and $y$ is the distance of the curve from the horizontal plane. This equation describes Euler’s elastica: equilibrium shapes of elastic rods, except that $\kappa$ 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, $\theta = d/ds$), 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, Euler’s Elastica on page 11

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

Figure 1. A knife balances stably on the edge of a full pot of water

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

Figure 3. Curvature $\kappa$ is caused by the pressure difference $p$ between the two sides of the water’s surface and is inverse proportional to the surface tension $\kappa = p/\sigma$. Since the hydrostatic $\rho g y$ (the excess of the air pressure over water pressure), we have

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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 SOL 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 bullpens.

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 course work. Careful reviewing of the work—perhaps redacting it in 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 persistence, creativity and curiosity 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 courses are available to assist with broadening programming 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 is also an adjunct professor in the Labour School of Business at the University of Wisconsin-Milwaukee.

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.

The Shape of Evolving Trees

[Extraction has played a major role in the history of life; after all, most species are extinct. Suppose we sample some subset X of species that are present today (species a–i 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 (phylogenetic trees often come in two forms: binary and non-binary). It turns out that under very general assumptions concerning the speciation-extinction process, many models predict an identical and simple discrete probability distribution on R(R(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 1/3 and 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 of two 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,...,n}, chosen uniformly at random. This is the YH probability distribution on R(R(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 according to a permutation on {1,2,...,n} (say, the “left-hand one” since the orientation in the plane plays no role) and let Zδ denote the number of leaves in this subtree. Remarkably, Zδ has a completely flat distribution.

Lemma 1. Zδ has a uniform distribution between 1 and n−1.

Proof: The random process Zδ,Zδ,..., is exactly what is a special case of a classical process in probability called Polya’s urn. This consists of an urn that at time 1 contains k red and n−k blue balls and at each time t, a ball is sampled uniformly at random and returned to the urn along with another ball of the same color. In our setting, a = n−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 Zδ 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 Polya’s urn with a = n−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 ∈ R(R(n)), the probability Pn(T) of generating T under the YH model is given by

\[ P_n(T) = \frac{1}{\binom{n}{n-1}} \prod_{j=0}^{n-2} \binom{Z_j}{Z_j}, \]

where V(T) is the set of interior vertices of T and λ(T) is the number of leaves of T that are descendants of v, minus 1. 

Curiously, a quite different process that arises in population genetics, and which 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.

Exercise: Find a general formula for the probability that a random tree T ∈ R(R(n)) generated by the YH model has the shape of a rooted caterpillar tree. What is the probability that T = F for a particular caterpillar tree F ∈ R(R(n))?

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 \( \theta = 0 \) as \( s \to -\infty \) and \( \theta = 2\pi \) as \( s \to +\infty \). This corresponds to heteroclinic solutions of the pendulum equation, with the pendulum approaching the unstable equilibrium in both future and past.

Derivation (1)

The force \( F \) is the weight of the lifted water of volume \( \pi RH \), where \( H \) is the maximal possible height (see Figure 3).

\[ F = \pi R^2 H. \]  

We must find the maximal possible \( H \) for which the surface tension can still keep the air film under the plate.

According to Figure 3, the equilibrium condition is

\[ 2R^2 \pi H = \pi R^2 H \text{LH} \]

After simple algebra, substituting \( \pi R^2 H \text{LH} \) into (4) yields

\[ H = \frac{2\pi R^2 \pi H \text{LH}}{2R^2 \pi H} \]

Substituting this value into (3) gives the lifting force (1). This is the theoretical maximum; the true value may be less because the angle \( \theta = \pi / 2 \) at the top is not zero, as is in Figure 3.

The figures in this article were provided by the author.

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Computational Topology in Geometric Design: Manifolds to Molecules

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

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 synthesizes 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].

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 topic [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 fuse-lages 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].

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 of each feature of 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 thus bridging (near the center of Figure 4) as structurally important.

Researchers developed special purpose algorithms to create responsive branched skeletons. They then 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 explored in the January/February 2020 issue of SIAM News.

Acknowledgements

Richard L. Anderson, David Bry, Michael A. Johnston, and William Swopo also made scientific contributions to this article. Kirk Gardner and Thomas J. Peters gratefully acknowledge generous financial support from IBM Research through its Open Collaborative Research and Shared University Research programs, by award IBM-TIP-0281403. Kirk Gardner and Donald R. Sheehy also appreciatively acknowledge partial funding from National Science Foundation (NSF) grant CCF-1652218. All statements in this article—including any errors—are the sole responsibility of these authors, not IBM Research or the NSF. All of the IBM and Science and Technology Facilities Council (STFC) teams were supported by the STFC Harwell Centre’s ‘Innovation Return on Research’ programme, which is funded by the U.K. Department for Business, Energy and Industrial Strategy.

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