Combining Data and Models to Study Woody Plant Encroachment

By Nathaniel A. Brunsell and Erik S. Van Vleck

Woody plant expansion into grasslands and savannas, which is accelerating worldwide, often affects ecosystem processes. Understanding and predicting the environmental and ecological impact of encroachment has led to a variety of methods for assessing its extent, transition, and stability. These methods generally rely on dynamical systems approaches. We seek to understand the competition between alternate stable states of grasses, trees, or shrubs and the influence of climate, fire, precipitation, and livestock grazing. Of particular interest to us are climate and fire interactions occurring worldwide (both naturally and due to fire suppression), especially the impact of woody encroachment on prairie grasslands in the central U.S. The Konza Prairie Biological Station (KPBS) is a native tallgrass prairie preserve located in the Flint Hills of northeastern Kansas, a grassland region of steep slopes overlain with shallow limestone soil unsuitable for cultivation. The Flint Hills region encompasses over 1.6 million hectares and is the largest remaining area of unplowed tallgrass prairie in North America.

The KPBS is divided into various watersheds, each with distinct enforced conditions. These conditions include different rates at which each watershed is burned and possible grazing by cattle or bison. The station is an ideal place to blend data acquisition and utilization with models to understand phenomena such as woody encroachment.

Our research on woody encroachment combines both data and models, and our initial efforts build on the development of simple low-dimensional stochastically-forced models [4-5, 7-8]. A low-dimensional model with stochastic precipitation and fire disturbance can examine the complex interactions between precipitation and fire as mechanisms that may suppress or facilitate increases in woody cover [1]. To analyze the impact of fire and precipitation frequency and intensity, we employ local in-time Lyapunov exponents or so-called Stoklov averages [2-3, 6] that assess convergence/divergence over different divergence time scales as a measure of relative stability or instability. Lyapunov exponents calculate the perturbation sensitivity of time-varying solutions of dynamical systems. By varying the parameters that

Self-organization in Space and Time

By Matthew R. Francis

Self-organization is an important topic across scientific disciplines. Be it the spontaneous flocking of birds or dramatic phase transitions like superconductivity in materials, collective behavior without underlying intelligence occurs everywhere.

Many of these behaviors involve synchronization, or self-organization in time, such as activation in heart cells or the simultaneous blinking of certain firefly species. Others are aggregations, or self-organization in space, like swimming shoals, flocking birds, or the alignment of electron spins in magnetic material.

Despite their conceptual similarity, self-organization in space and time have largely been treated separately. “I was curious about whether the two fields had been wedded, and it turns out they hadn’t, at least not fully,” Kevin O’Keeffe, a postdoctoral researcher at the Massachusetts Institute of Technology, said. “I knew all these tricks and mathematical tools from synchronization, and I was looking to cross-fertilize them into the swarming world.”

O’Keeffe, along with Hyunsuk Hong of Chonbuk National University in South Korea and Steven Strogatz of Cornell University, developed a simple model for circadian rhythms based on interacting oscillators. A few years later, physicist Yoshiki Kuramoto developed a related model and solved it exactly. Researchers have created many variations of the Kuramoto model to address everything from firefly flash synchronization to superconductivity; it is also similar in mathematical form to several physics-based models of magnetism.

O’Keeffe and his team based the swar- malator model on the simplest form of the Kuramoto model: a system of coupled ordinary differential equations (one for every oscillator) that each oscillator interacts with all others at the same strength — there is no falling off with distance or communica- tion time lag, for example. A single (scalar) parameter sets both the strength of the interaction and the system’s preference as to whether all the oscillators are in or out of phase. The phase system cycles freely when the parameter is zero, much like the minute hand of a clock revolving at a steady rate of one cycle per hour.

As a general rule, swarming is much more complicated than synchronization. It is easy for two systems to find three directions in space but only one in time. If the swarming bodies are free to move in all three directions, they have many possible ways to self-organize.


Self-organization in Space and Time
It’s a Matter of Style

Does your writing have a noticeable style? Is there something characteristic about your use of vocabulary, punctuation, voice, and the many other ingredients of written composition?

Style is like a piece of music on your mind when you are writing a paper. Refining and verifying the technical content and completing the paper are usually of higher priority. Although the format of an academic paper is quite rigid and confining, there is still plenty of scope for writing it your own way. A trivial example is the explanation of a paper’s organization, which usually appears at the end of the introduction. Many authors write, “The contents of this paper are as follows,” or “The rest of this paper is organized as follows.” But there are ways to avoid these clichéd phrases. For example, one can write, “We begin, in the next section, by...” The ensuing sentences are typically of the form, “In section 2 we investigate...” — you could rewrite these more compellingly to sound less like a table of contents. How you cite other work is also very much a matter of style. Companies like Elsevier are conscious of this and will often insist that you use their house style.

Somebody Else’s Dream

Bonita Saunders gives an inspiring account of her road to a career as a research mathematician at the National Institute of Standards and Technology. As a young African American student, she experienced the complicated aftereffects of school integration firsthand.

Research Software Engineer: A New Career Track?

Chris Richardson and Mike Croucher outline a U.K. initiative spearheaded by the Software Sustainability Institute to improve academic software reliability and reusability by encouraging better software practices and pushing for a unique research software engineering career track, the institute is enhancing research software in academia.

Jupyter: Tools for the Life Cycle of a Computational Idea

Mini Regina-Kelly, Carol Willing, and Jason Grout provide an overview of Project Jupyter, a software platform from interactive exploration and experimentation to publication and communication of results—for the life cycle of a computational idea.

8 The Underlying Laws Binding Cities, Companies, and Living Systems

James Case reviews Scale: The Universal Laws of Growth, Innovation, Sustainability, and the Pace of Life in Organisms, Cities, Companies, and Civilizations, a book written by Geoffrey West, who argues that one can apply the basic laws of physics that define growth in the physical world to the biological, political, and corporate realms.

12 Reservoir Computing: Harnessing a Universal Dynamical System

When a dynamical system, a set of coupled differential equations, is in a regime of high nonlinearity, it can act as a reservoir that is capable of processing signals like weather forecast- ing and radio transmitter fingerprinting. Daniel J. Gauthier describes how a reservoir computer can train a “universal” dynamical system to predict the dynamics of a desired system.

FROM THE SIAM PRESIDENT

By Nicholas Higham

A different aspect of style is the house style of journals. Most reputable journals have a prescribed submission style for uniformity. Copy editors edit for this style and correct grammatical and formatting errors in manuscripts. SIAM is well known for the quality of its copy editing. Less well known is the SIAM Style Manual, which is freely available.1 SIAM style is not too prescriptive and largely follows standard guidelines, such as those in the Chicago Manual of Style, though with more detail on how to format mathematics. Among the advantages of conforming SIAM style for copy editors, the SIAM Style Manual is also an informative read for good exercise. You might as well try to adhere to the style guidelines if you are writing for a SIAM journal as this will minimize the copy editing changes made to your manuscript. More specifically, thinking about style issues may help you improve your paper’s readability.

Less experienced authors who submit to SIAM may benefit from improved wording provided by SIAM copy editors — as many of us have over the years, and as Knuth did from the TAOCP copy editors. Likewise, my articles always benefit from improvements suggested by SIAM News copy editors, who apply SIAM News’s own house style.

Another aspect of style concerns the LaTeX style file used to produce SIAM papers. This has evolved over the years, with a major modernization in 2016.2 The most recent version is dated December 17, 2017, and is thoroughly documented. It comes with a BibTeX style file siamplain.bst that formats your bibliography in SIAM style, and will include DOIs if they are present in the bibliography database. By using siamplain.bst, you can produce a neatly formatted, DOI-linked bibliography and save a great deal of copy-editing time.

References


Nicholas Higham is the Richardson Professor of Applied Mathematics at The University of Manchester. He is the current president of SIAM.
Modelling Drug Dynamics in the Brain

By Vivi Rottschäfer

While scientists have devoted much research to models of neural activity in the brain, they have paid little attention to modeling drugs that target the brain. Development of this class of drugs is very challenging and necessitates an understanding of the highly complex processes that govern the concentration profile of a drug in the brain over time. Since access to the brain for measurement purposes is very limited, a mathematical model is a helpful tool. But before we present a model, we must introduce some of the brain’s physiology and the processes that occur after medication consumption.

The brain is interlaced with a network of blood capillaries (see Figure 1). Following intravenous or oral administration and subsequent intestinal absorption, the drug in question begins to circulate in the blood and primarily enters the brain from the arterial network by crossing the blood-brain barrier (BBB). One of the BBB’s principal functions is to limit transport into the brain and protect it from harmful substances, thereby preventing brain damage. When the drug does enter the brain through the BBB it circulates in brain fluids, such as the extracellular (ECF) and cerebrospinal (CSF) fluids. It then binds to receptors on cells of the BBB’s principal functions is to limit transport into the brain and protect it from harmful substances, thereby preventing brain damage. When the drug does enter the brain through the BBB it circulates in brain fluids, such as the extracellular (ECF) and cerebrospinal (CSF) fluids. It then binds to receptors on cells (see Figure 2, on page 1). When a drug binds to a receptor, it leads to an effect in the body. Here we will focus on drug transport in ECF and the subsequent binding to receptors.

Compartmental models are widely used in pharmacology, and have also been developed to model drug concentration in the brain. For example, [1] presents a general compartmental model of the central nervous system. Unfortunately, these models do not account for drug transport in ECF and other tissues, which mainly occurs via diffusion and bulk flow. Moreover, compartmental models do not consider receptor binding. A diffusion-advection equation can model drug transport where the drug is administered directly into the brain [2].

As a first step towards a full model of the brain, our model incorporates diffusion and flow in ECF, inflow through the BBB, and receptor binding.

Though the brain is three-dimensional, we start by creating a model on a two-dimensional domain, which represents a tissue unit of brain ECF. This square domain is surrounded by brain capillaries and can be considered the smallest building block of the brain, in terms of drug distribution (see Figure 3). In the human brain, the distance between capillaries is on average 50µm. Cells with receptors are located inside the domain. We model drug transport in the unit by diffusion and bulk flow, assuming that the latter occurs in the z-direction. One can consider ECF a porous medium, as it is filled with many obstacles—such as cells and proteins—that limit diffusion. This leads to an effective diffusion smaller than normal (in a medium without obstacles). We model this with the so-called tortuosities λ, thereby dividing the normal diffusion by λ, which results in a smaller diffusion coefficient. Tortuosity differs between drugs due to their varying sizes and deformabilities. To formulate the model, we denote the concentration of free (unbound) drug by D.

The equations for N swarmalators are

\[
\dot{x}_i = \sum_{j=1}^{N} \left[ \frac{1}{N} (1 - J \cos (\theta_i - \theta_j) - \theta_i) - \frac{x_i}{\theta_i + \theta_j} \right] K \sin (\theta_i - \theta_j),
\]

where the dot indicates an ordinary differential equation with respect to time. Because the swarmalators begin in a state with no oscillations or motion in space, the initial conditions for the system are static.

The coupling parameter K, modulated by the distance between the swarmalators, determines how strongly the oscillator state synchronizes. When K is positive, the oscillator states minimize their phase differences. When K is negative, the phase difference grows with distance across the swarm. Swarmalators settle into a static ring pattern in space. This is qualitatively similar to the behavior of colloidal particles on a surface, where the oscillator variable corresponds to the electro-dipole of the particles. (d) Keeping J > 0 and looking at small negative K values produces something O’Keeffe jokingly calls a “pizza” configuration, which is analogous to a wave. This is like a sports wave, with significant divisions between each group of fans’ motion. (e) The translational state between phases (b) and (d) creates a system of groups of counter-rotating swarmalators. This is qualitatively similar to sperm behavior, where the ‘wiggling tail’ represents the oscillations. The cells tend to stick to surfaces and create clusters in which all the sperm wiggle their tails synchronously, but neighboring clusters have slightly different oscillation phases. Despite its simplicity, the swarmalator model exhibits enough complex behavior to be interesting. Simplicity often means generality, and extending the original model can provide ways to restore any lost specificity. You want the simplest model that gives you the right physics,” O’Keeffe said. “That is why the Kuramoto model took off and became so popular — just because it was simple.”

There is still much to learn from the model as it stands. For instance, the equations give ambiguous results — analogous to water freezing or a material becoming magnetized — knowledge of them is important for understanding the function of swarmalator groups.

O’Keeffe hopes other researchers will further study the system. “The dream would be to get some experimentalists or physicists interested in this, who could engineer real swarmalator systems,” he said. “If someone could go out there and come up with something tangible, that would be brilliant.”

References

Further Reading


Matthew R. Francis is a physicist, science writer, public speaker, educator, and frequent wearer of dusty huts. His website is BowlerHatScience.org.

Figure 1. The brain and its interlacing capillary network. (a) The brain. (b) The network of capillaries that intertwines the brain. (c) Brain capillaries from the human cerebral cortex. Images 1a and 1b are public domain images, and 1c is courtesy of [1].

Figure 2. The two-dimensional unit of extracellular fluid, which contains cells with receptors and is bounded by blood capillaries. Concept for figure provided by Vivi Rottschäfer.

Figure 3. The three-dimensional unit of extracellular fluid, which contains cells with receptors and is bounded by blood capillaries.
Plant Encroachment
Continued from page 1

control fire and precipitation, and comparing the dependence of quantities analogous to the largest Lyapunov exponent as a function of these parameters, we ascertain the relative control exerted on woody encroachment through these mechanisms.

Researchers have successfully employed the largest Lyapunov exponent in different areas of biology and ecology as an indicator of chaos (sensitivity to initial state) and a measure of the relative sensitivity of parameterized systems. For example, Lyapunov exponents are indicative of a dynamical system’s exponential rate of change either away or toward a particular state of the system, such as a grass or woody state. A positive exponent indicates a predicted rate away from the current state, i.e., an unstable state and transition to a stable one. A negative exponent indicates a trajectory toward the initial state, meaning that the state is stable. Therefore, if a given precipitation environment results in a negative Lyapunov exponent for woody fractions, the particular rainfall regime is stable for the expansion of woody species; a positive exponent signals an unstable regime.

Figure 1 displays the divergence time $t$ versus the logarithm of divergence distance $\|x(t) - x(0)\|_2$ (time-averaged logarithm, defined by $\log_t \left( \frac{1}{t} \sum_{i=1}^{t} d(\tau_i) d(\tau_{i+1}) \right) \approx \log_t(1 + t)$, where the average is over $j$ and $d(\cdot)$ denotes the divergence of the $\chi^2$ difference over a fixed length of time $t$. $\chi^2$ is analogous to the largest Lyapunov exponent here. $\chi^2$ describes the divergence average over time intervals of length $i$. The algorithm in [6] allowed for computations using an appropriate delay coordinate embedding. Figure 1 illustrates the behavior of the normalized local Lyapunov exponents for a subset of the precipitation magnitude, frequencies, and burned considered in [1] that corresponds to a 16-year fire frequency and high annual precipitation.

Next steps involve the incorporation of data into more complex land surface models (LSMs). Noah-mp is an LSM that employs multiple options for key land-atmosphere interaction processes. It contains a separate vegetation canopy defined by a canopy top and bottom, crown radius, and leaves with prescribed dimensions, orientation, density, and radiometric properties. The Noah-mp model prescribes both the horizontal and vertical density of vegetation using either ground- or satellite-based observations. It utilizes a dynamic vegetation model that allocates carbon to various parts of vegetation (leaf, stem, wood, and root) and soil carbon pools (fast and slow). The model distinguishes between C3 photosynthetic pathways (used by most plants) and C4 pathways (used more by semi-arid grasses), and defines vegetation-specific parameters for plant photosynthesis and respiration.

To understand transitions between these competing stable states, we are interested in quantifying some form of coupling metrics from Ameriflux data, remotely-sensed atmospheric profiles, atmospheric boundary layer height and soil moisture, and output from both a low-dimensional model and the Noah-mp model. These factors will help identify the coupling structure and relationship to available energy and partitioning, vapor pressure, and temperature gradients to quantify each state’s stability and determine the underlying data and model sensitivity. Ultimately, this will increase our understanding of the physical mechanisms responsible for coupling dynamics in the central U.S. Stabilization Frequency is more significant than the largest Lyapunov exponent as a function of the divergence time scale. Figure 1 also shows that these local type exponents produce an annual pattern with seasonal variations for some parameter configurations. Grass assimilation (A), woody transpiration (Trw), and top layer soil moisture ($\theta$) have two peaks over year while various others—such as bare soil evaporation (E)—have one peak per year. Two peaks in these plots correspond to instability (sensitivity with respect to perturbations in that variable) over divergence times of zero-three months, six-nineteen months, 12-15 months, etc.; one peak per year corresponds to instability over divergence times of zero-six months, 12-18 months, etc. Perturbations are amplified by approximatively $e^{\alpha t}$ so that they grow with time when the slope in Figure 1 is positive and decay when the slope is negative.

The results in [1] indicate that precipitation frequency is more significant than the intensity of individual precipitation events when controlling woody encroachment. Fire, however, has a much more dominant impact on limiting encroachment. These results suggest that fire management—in the form of more frequent burns—may be an effective strategy to slow the onset of woody species into grasslands. While climate change might predict a reduced potential for woody encroachment in the near future, these findings imply that a reduction in woody fraction may be unlikely when considering anthropogenic fire suppression.

Recent Advances in Dimensionality Reduction with Provable Guarantees

The following is a short introduction to an invited lecture to be presented at the upcoming 2018 SIAM Annual Meeting (AN18) in Portland, Ore. from July 9-13. Figure 1 also shows that these local type exponents produce an annual pattern with seasonal variations for some parameter configurations. Grass assimilation (A), woody transpiration (Trw), and top layer soil moisture ($\theta$) have two peaks over year while various others—such as bare soil evaporation (E)—have one peak per year. Two peaks in these plots correspond to instability (sensitivity with respect to perturbations in that variable) over divergence times of zero-three months, six-nineteen months, 12-15 months, etc.; one peak per year corresponds to instability over divergence times of zero-six months, 12-18 months, etc. Perturbations are amplified by approximatively $e^{\alpha t}$ so that they grow with time when the slope in Figure 1 is positive and decay when the slope is negative.

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Drug Dynamics

Continued from page 3

and active transport, we only analyse pas-
sive transport resulting from diffusion. At
x = 0, this leads to

\[
\frac{dD(B)}{dt} = P(D - D_{BBB}(t)),
\]

and similar conditions at the other bound-
aries [4]. P is a measure of the perme-
ability—transport through the BBB—and
\(D_{BBB}(t)\) describes the drug concentration in the surrounding capillaries’ blood. This can and will vary with time since the drug enters the blood and is thereafter eliminated from it.

The time dynamics of the concentrations is of interest, and this presents an important mathematical challenge. We begin by focusing on the “standard” question of behaviour of solutions as t becomes large; at t = 0, all of the drug is eliminated from the brain. We perform simulations, study the free drug concentration and the bound com-
plex concentration in the domain over time [4], and choose all coefficients in physically-relevant ranges. Many of the coefficients vary widely among different drugs. Therefore, we examine the influence of changing various parameters on the concentration. As an example, we show results of simulations where we kept \(D_{BBB}(t)\) and permeability \(P\) on the concentration. After fixing the rest of the parameters and only changing \(D_{BBB}(t)\), we see plots of the free drug D and bound drug B versus time in the middle of the domain (see Figure 4). We also plot the concentration of drug in the blood \(D_{BBB}(t)\) (in red).

We vary \(P\) from the lowest possible physiological value to an intermediate, fol-
lowed by a larger value. The lowest value meant emulating my superb elementary and high school education in Portsmouth, Va., in the 1960s and 70s, that I also wanted to be a career. As a young girl growing up in Portsmouth, Va., in the 1960s and 70s, that meant emulating my superb elementary and high school teachers. However, teaching was considered a prestigious and lucrative career to which most African Americans aspired, and it attracted some of the best and brightest minds.

I was born shortly after the landmark Brown v. Board of Education Supreme Court decision, which declared laws specifying “separate but equal” education unconstitutional. In the early 60s, Portsmouth implemented the “Freedom of Choice,” a policy that allowed students to attend any public school in the city. This typically meant that a few black students attended white schools, but no white students attended black schools. Like most black students, I continued to attend black schools. But by the early 70s, the threat of court cases pressured many school systems—including Portsmouth—to abandon their failed integration policy and implement busing.

Figure 4. A two-dimensional grid around an airfoil, or wing cross section. The area near the tips, at the root, and at the washout, the large concentration of grid points needed to solve the Navier-Stokes equations is evident. Farther away from the wing, the airflow is less affected and fewer grid points are needed. Figure credit: Bonita Saunders.

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pound concentration in the domain over time [4], and choose all coefficients in physically-relevant ranges. Many of the coefficients vary widely among different drugs. Therefore, we examine the influence of changing various parameters on the concentration. As an example, we show results of simulations where we kept \(D_{BBB}(t)\) and permeability \(P\) on the concentration. After fixing the rest of the parameters and only changing \(D_{BBB}(t)\), we see plots of the free drug D and bound drug B versus time in the middle of the domain (see Figure 4). We also plot the concentration of drug in the blood \(D_{BBB}(t)\) (in red).

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Research Software Engineer: A New Career Track?

By Chris Richardson and Mike Croucher

In 1675, Isaac Newton famously wrote in a letter to Robert Hooke, “If I have seen further, it is by standing on the shoulders of giants. Perhaps I was not being entirely kind to his colleague and rival, but the general idea pervades the sciences to this day: we rely on others’ work to advance our own. This has never been truer than in the world of research software.

Software written for academic purposes has a poor reputation for reliability and reusability. It is not uncommon to hear about a newly-developed software in one’s research area, only to find that it has no documentation, does not compile on all systems, yields errors, or is out of date. Given the lack of incentive for academics to devote precious time to write documentation, test code on other systems, or even keep it working, this is no surprise. Once researchers have found solutions to their specific questions and published a few papers with their code’s outputs, there is little reason for anyone to advance software developed for this purpose.

Recognising this problem, several like-minded individuals at the University of Southampton, the University of Oxford, and the University of Manchester came together in 2010 to form the Software Sustainability Institute (SSI). With the tagline “better software, better research,” they have been promoting “software carpentry,” collaborations workshops, and sponsored software conferences in the U.K. An SSI survey found that 70 percent of researchers relied on software for their results, and over 50 percent wrote their own software. By advocating for revision control, automated testing, and open-source development, SSI’s founders have significantly impacted research software, both in the U.K. and internationally. However, it soon became clear that encouraging better research software practices could only produce limited results, as most academics had very little time to focus on it. Those that did were failing to advance in their careers because they had spent too much time producing software for everyone else’s benefit.

While Newton was able to give up his theological studies to devote himself to the new field of science, most researchers do not have the luxury of abandoning publication to concentrate on software development. The SSI leadership realised that the best way to improve software quality was to invent a new career track with a different set of metrics. The term “research software engineer” (RSE) was coined at an SSI-sponsored event to describe a career track which was typically devoted to software within the research community. In January 2014, the U.K. Research Software Engineer (UKRSE) Association was formed to provide advice and guidance to anyone who identifies as an RSE. The association is free to members. Around this time, a few U.K. universities began experimenting with “research software groups” (RSGs) — teams comprised of programmers not dedicated to any specific project, but instead available as resources across the university. Providing a mechanism to interact with academics and conduct the maintenance, testing, and documentation that otherwise would not occur has produced better-quality software. The experiment was a success, and the model has spread across the country.

As of March 2018, the SSI leadership reasoned that the best way to improve software quality was to found an international RSE community. In May 2018, the Research Software Group (RSG) was launched. Its first goal was to identify the barriers to entry for researchers new to the RSE field by surveying 106 researchers across the globe. The SSI experiment was a success, and the model has spread around the world.

The SSI leadership reasoned that the best way to improve software quality was to invent a new career track with a different set of metrics. The term “research software engineer” (RSE) was coined at an SSI-sponsored event to describe a career track which was typically devoted to software within the research community. In January 2014, the U.K. Research Software Engineer (UKRSE) Association was formed to provide advice and guidance to anyone who identifies as an RSE. The association is free to members. Around this time, a few U.K. universities began experimenting with “research software groups” (RSGs) — teams comprised of programmers not dedicated to any specific project, but instead available as resources across the university. Providing a mechanism to interact with academics and conduct the maintenance, testing, and documentation that otherwise would not occur has produced better-quality software. The experiment was a success, and the model has spread across the country.

Of course, nothing happens without funding. The funding model adopted by most research software groups involves requesting a core set of positions and services with central university funds. Academics can then access this pool of resources by including an RSE element in their grant proposals, which is then charged back to the RSE pool. This model helps universities retain talented RSEs and provides both additional flexibility for academics and a stable career pathway for the RSEs themselves.

https://www.software.ac.uk

References


Bonita Saunders is a research mathematician in the Applied and Computational Mathematics Division at the National Institute of Standards and Technology. She is the secretary for the SIAM Activity Group (SIAG) on Geometric Design, and webmaster and mailing list moderator for the SIAG on Orthogonal Polynomials and Special Functions.

3 http://dlmf.nist.gov/

4 http://dlmf.ac.uk/community/research-software-groups/rssg/

5 https://www.software.ac.uk

Figure 1. A Digital Library of Mathematical Functions (DLMF) webpage with an embedded visualization of the Reimann zeta function, an important function that arises in the field of number theory (left). Computing the function value at each point on the grid (right) provided the surface data that was used to create a color map. Figure credit: Bonita Saunders.

Figure 2. A Digital Library of Mathematical Functions (DLMF) webpage with an embedded visualization of the Reimann zeta function, an important function that arises in the field of number theory (left). Computing the function value at each point on the grid (right) provided the surface data that was used to create a color map. Figure credit: Bonita Saunders.

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Somebody Else’s Dream

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At NASA’s Langley Research Center. This eventually led to a graduate student research fellowship at NASA that paid more than my teaching position at Hampton. My research involved boundary-fitted grid, or mesh, generation. Such grids are used in fields where equations are solved over an oddly-shaped domain, such as aerodynamics (aircraft, automobile design), hydrodynamics (ship design), electromagnetics, and materials science. Figure 1 on page 5 shows a grid constructed via variational methods and tensor product B-splines that may be used to enhance my computer skills. But provided an excellent opportunity to facilitate the plotting of function surfaces containing branch cuts, zeroes, poles, and other areas of interest (see Figure 2). I created a sub-project supported by a dedicated team of both NIST computer scientists and mathematicians, and college students employed under NIST’s Summer Undergraduate Research Fellowship internship program. We created more than 600 graphs and visualizations of complex functions while also advancing research in interactive three-dimensional web graphics. Over a decade of work has led to numerous technical publications and presentations at international conferences. The DLMF Project team has received several awards and honors, including a U.S. Department of Commerce Gold Medal (2011); a cover article in Notices of the American Mathematical Society (August 2011); and recently, an invited article in Physics Today, the flagship publication of the American Institute of Physics [3]. I serve on the DLMF editorial board and also lead one of several spinoff efforts, the NIST Standard Reference Tables on Demand Project. The project is a collaboration between NIST’s ACM and the University of Amwer’s Computational Mathematics Group to build an online testing service where users can generate high-precision tables of special function values with certified error bounds for comparison with their own uploaded function data.

So why do I feel like I’m living somebody else’s dream? Well, my career bears little resemblance to the dream I initially described. But fortunately, I’ve had some time to reflect on a hasty comment made during a pensieve mood. What was I thinking? Of course I’m living somebody else’s dream! I’m living the dream of Hidden Figures Mary Jackson, who reluctantly gave up her engineering career to accept a position as an equal employment opportunity manager to advance the careers of other women and minorities; the dream of my excellent first-grade teacher, who longed for the chance to be excellent in another career; the dreams of my parents, who graciously viewed my accomplishments as a reflection of their dreams of civil rights legends like Congressman John Lewis, who have lived to see the heirs to their dreams. And may I never forget: the dreams of countless slaves, whose only freedom was their dreams.

https://www.nist.gov/summer-undergraduate-research-fellowship-surf

http://dlmf.nist.gov

http://dlmf.ac.uk/community/research-software-groups/rssg

https://www.software.ac.uk

2 http://dlmf.nist.gov/

1 http://dlmf.nist.gov/
Jupyter: Tools for the Life Cycle of a Computational Idea

By Min Ragan-Kelley, Carol Willing, and Jason Grout

Computation is increasingly becoming an integral part of science and education across disciplines. The life cycle of a computational idea typically involves interactive exploration and experimentation, as well as publication and communication of results. Reproducible computation demands open research tools, good software practices, and transparent documentation of research processes and results. Project Jupyter\(^1\) is an open community that builds open-source software tools and protocols for the life cycle of a computational idea. Two core pieces of the project are an open protocol for interactive computation and an open document format with which to record and share computational ideas. The Jupyter Notebook application builds on these to provide a powerful, interactive, computational environment.

### The Jupyter Notebook

**What Is a Notebook?** The Jupyter Notebook is a document composed of a sequence of code cells and markdown cells. A code cell contains a block of code (in any language, including but not limited to Julia, R, and Python) and the output from running the code. Output displayed below a code cell is a rich representation of results and can include text, images, and interactive visualizations. A markdown cell consists of prose text in the markdown format—a lightweight, shorthand syntax for HTML—with added support for LaTeX mathematics. This structure allows authors to interface formatted narrative and mathematics with blocks of code and their rich outputs, rendering the notebook document a powerful tool for communicating insights and results.

The notebook document format is free, open, and transparent, in keeping with its aim to facilitate open and accessible science. It is stored as a single JSON-formatted text file, making it easy to manipulate and understand using standard programming tools, without the need for Jupyter software. The notebook file format is public\(^2\) and Jupyter software is open source under the BSD license.

Many authors communicate using Jupyter Notebooks. GitHub hosts 1.4 million notebooks, and some people have written entire books as collections of notebooks, such as Jake Vanderplas’s Python Data Science Handbook.\(^3\) Because notebook documents preserve their content structure and metadata, they are easily convertible to other formats, including plain scripts in LaTeX, Markdown, and reStructuredText via Jupyter’s conversion tool, nbconvert.\(^4\)

Using Notebook Documents. The Jupyter Notebook server is a web-based application for interacting with notebook documents. The server renders the notebook for the user and begins a persistent interactive ‘kernel’ session in the desired language (such as Julia, Python, R, etc.) for executing user code. A user enters the code in a code cell and runs it (in the kernel session) before viewing the rich output results from the kernel, which may include text, images, and interactive controls. The user continues creating, editing, and executing or re-executing code cells and markdown cells. The user can also create down cells to explain how the code to execute and the resulting rich visualizations. A markdown cell consists of prose text in the markdown format—a lightweight, shorthand syntax for HTML—before adding LaTeX mathematics. The kernel protocol—a transport layer for interactive computation through the Jupyter Message Protocol—enables Jupyter kernels and notebook files. GitHub\(^5\) and nbviewer\(^6\) render notebook files for read-only viewing online. By building on the Jupyter software, the Jupyter Notebook application integrates with other computational tools has evolved for interactive computing. Computational environments such as JupyterLab\(^7\) (the successor of the Jupyter Notebook application, see Figure 2 on page 9), the JupyterHub, and notebook applications and notebooks, and some people have written entire books as collections of notebooks, such as Jake Vanderplas’s Python Data Science Handbook.\(^3\) Because notebook documents preserve their content structure and metadata, they are easily convertible to other formats, including plain scripts in LaTeX, Markdown, and reStructuredText via Jupyter’s conversion tool, nbconvert.\(^4\)

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Several funding councils have supported this model, with the U.K.’s Engineering and Physical Sciences Research Council (EPSRC)\(^8\) taking the lead. EPSRC provided the initial funding for the SSI (subsequently joined by the Bioinformatics and Biological Sciences Research Council and the Economic and Social Research Council), along with funds for a fundamentally different type of research fellowship—the RSE Fellowship.\(^9\)

The EPSRC RSE Fellowship scheme has funded over 11 fellows across two funding calls, thus far. The programme funds each individual for a five-year period and offers participants a great deal of freedom to develop as leaders in their institutions. Projects are highly varied and include development of specialised software, establishment of RSEs and national RSE networks, exascale and accelerator-based computing, data visualisation, and diverse training programs.\(^10\)

The right solution may take some time. Ultimately, RSE advancement in the U.K. has been a great success so far.\(^11\) The UKRI Science and Industry in Manchester, U.K., in September 2017. The meeting brought together RSEs from 14 different countries, including many in Europe, and as far as Canada and New Zealand.

Chris Richardson has spent time in physics, mathematics, and geosciences departments in the U.K. and Japan, and now works at the University of Cambridge as a research software engineer. He is a core developer in the open-source ENSCI (Exascale scientific code, and an Engineering and Physical Sciences Research Council (EPSRC) Research Software Engineering Fellow. Mike Croucher is also an EPSRC Research Software Engineering Fellow and co-founder of the Research Software Engineering Group at the University of Sheffield. Beginning in April 2018, he will be director of research computing at the University of Leeds.


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The Underlying Laws

Binding Cities, Companies, and Living Systems


A s a teenager in London, physicist and author Geoffrey West procured a temporary job in the research labs of International Computers Limited. It was a transformative experience, during which he decided to pursue a career in research. After obtaining an undergraduate degree in physics at the University of Cambridge and a Ph.D. from Stanford University, West eventually moved to Los Alamos National Laboratory and became the founder and group leader of the Elementary Particle Physics and Field Theory Group. He later joined the Santa Fe Institute (SFI), eventually serving a term as president. In 2006, he was listed among Time’s “100 Most Influential People in the World.” Among the phenomena that initially piqued West’s interdisciplinary curiosity were the extraordinary number of documented power laws \( y \sim x^p \), which reduce to straight lines when both variables are measured on a logarithmic scale. He possesses a physicist’s appreciation of scaling arguments, and traces the development thereof—from Galileo—who argued that the heights to which certain animals can grow is limited by the fact that areas increase as the square of height while volumes increase as the cube—to William Froude—who discovered the importance of the ratio \( \frac{1}{2} \rho V^2 L \) for ship design—to Lord Raleigh, who explored the advantages of expressing physical laws in terms of dimensionless variables. Scale’s main story line—from which West digresses early and often—begins with four striking power law examples, illustrated by scatter plots of the following: the basal metabolic rates of animals against their body mass, the number of patents held by residents of particular cities against their populations, and the income and/or assets of corporations against the number of their employees. The basal metabolic rate of an organism is simply the rate at which it consumes energy while at rest (for such, \( p \approx 3/4 \)). For heartbeats in a lifetime, \( p \approx 0 \), indicating that the hearts of virtually every known species beat roughly one billion times between birth and death. Small animal hearts beat much faster than human hearts, while large animal hearts beat more slowly. Thus, dogs and cats live only a few short years, while whales and elephants live many times longer than humans. The fact that \( p \approx 3/4 \) for metabolic rates implies an economy of scale whereby an animal weighing 100 times as much as another consumes only 32 times as much energy while both are at rest. For patents held by city residents, as for income and/or assets of corporations, \( p \) exceeds unity, meaning that a city or firm that is 100 times as large as another consumes more than 100 times as many resources. Therein, says West, lies a fundamental difference between biophysical and socioeconomic growth. As intriguing as the ubiquity of power laws themselves is the tendency of the observed exponents \( p \) to cluster, at least in the biophysical realm, around multiples of 1/2. Where \( g \) is acceleration due to gravity, \( V \) is velocity, and \( L \) is the length of the vessel of interest.

Figure 1. Geoffrey West’s universal growth curve. Courtesy of Penguin Press.
The Mathematics of Wrinkles and Folds

The following is a short introduction to an invited lecture to be presented at the upcoming 2018 SIAM Annual Meeting (AN18) in Portland, Ore., from July 9-13. Look for feature articles by other AN18 invited speakers introducing the topics of their talks in future issues.

The wrinkling and folding of thin elastic sheets is familiar to most: our skin wrinkles, a crumpled sheet of paper folds, and a flat sheet stretched over a round surface must wrinkle or fold. Similar patterns occur in a wide variety of settings. Their study is important for a number of reasons: (a) In some situations, wrinkling patterns are highly ordered and reproducible. Such patterns can be useful when measuring the physical properties of sheets or designing templates for self-assembly, for example. (b) Wrinkled configurations are local minima of a variational problem—the elastic energy of the sheet—with a rather special structure. Understanding their properties is a problem in energy-driven pattern formation, a current frontier in the calculus of variations. (c) We would like to understand the features of low-energy configurations in specific settings; this will help us separate universal phenomena from those that depend, for example, on the history of loading. (d) Strong analogies exist between the wrinkling of elastic sheets and pattern formation in other physical systems, such as liquid crystals, ferromagnets, and superconductors. Progress in any of these areas has the potential to yield insight for the others. What kind of mathematics is this? The elastic energy of a thin sheet consists of a nonconvex membrane energy (which prefers in-plane symmetry) plus small coefficient times bending energy (which penalizes curvature). The bending term is a singular perturbation; its small coefficient is the sheet thickness squared. The patterns and defects in thin sheets arise from energy minimization—but not in the same way that minimal surfaces arise from surface area minimization. Rather, analysis of wrinkles and folds involves the asymptotic character of minimizers in the limit as the sheet thickness tends to zero. What kind of methods are useful? Simulation is of limited utility, since the problems are highly nonconvex and very stiff. Bifurcation theory is also of limited utility, because the configuration of interest lies deep in the bifurcation diagram. Instead, focusing on the energy scaling laws—the minimum energy’s dependence upon the thickness of the sheet (and other relevant physical parameters)—has been fruitful. Optimizing the energy within a particular ansatz gives an upper bound on the minimum energy. Obtaining ansatze-free lower bounds is a key mathematical challenge. The lower and upper bounds are useful for comparing the theoretical predictions to simulation.

Jupyter

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same Jupyter formats and protocols, the aforementioned variety of interoperable tools enables interdisciplinary collaboration and communication among researchers, students, and others.

Reproducible Scientific Results

Jupyter provides useful tools for communicating scientific results. At its base level of reproducibility, a notebook is a single, shareable document containing a prose explanation of an idea, code for its implementation, and the output and figures illustrating the results. To accurately reproduce another researcher’s findings, a reader needs access to a similar computational environment, including the applicable data and software libraries. Binder15 provides a service for sharing a reproducible computational environment. For example, the LIGO/Virgo collaboration (see Figure 3) uses Binder to enable interaction with its Nobel Prize-winning research, observing gravitational waves with a single click.16

Enhancing Education

Due to its strength in exploratory research and scientific communication, Jupyter has found a welcome home in education. As computation becomes more prominent in various academic fields—including computational biology, digital humanities, and data science—in education, Jupyter has become more prominent in ever-widening fields—including computational biology, digital humanities, and data literacy—almost every student will need to apply programming in some form. Several open-source tools for educational development around the Jupyter Notebook.

RISE,17 a plugin for the Jupyter Notebook application, displays and runs code as presentations by stepping through interactive content. These presentations are live notebooks, so instructors can pause to answer questions and run code demonstrations. The nbgrader project18 is another example of a tool that is useful to educators. It allows instructors to automatically distribute Jupyter Notebook assignments and students to submit completed notebooks. Since notebook cells sometimes have associated metadata, instructors can mark submissions efficiently by selecting certain notebook cells to be automatically graded and others to be graded by hand.

Conclusion

Project Jupyter provides open, documented protocol and notebook file format standards, in addition to a wide variety of interoperable open-source tools for the life cycle of a computational idea. These open standards and tools range from early exploratory interactive research to communication of insights and results, and enable a flourishing ecosystem to support collaboration and reproducibility in science and education.

Acknowledgments:
The authors wish to recognize the following people for their contributions to this article: Fernando Perez, Paul Ivanov, Brian Granger, Jessica Forde, Matthias Bussoni, and Damian Avila, as well as the Project Jupyter team on whose combined work this report is based.

Min Bk Kang-Kelley has been working on interactive computing tools as part of the IPython and Jupyter teams since 2006. He now works primarily on IPythonHub as a postdoctoral researcher at Simula Research Laboratory in Oslo, Norway. Carol Willing is a Python Software Foundation Fellow and former director, a core developer of Cython and Project Jupyter, and a research software engineer at California Polytechnic State University. She is also a Flight Researcher at Nasa. She has been helping develop open-source scientific software platforms, such as SageMath and Jupyter, since 2007.

Figure 2. View of a notebook GeoJSON file in JupyterLab.

Figure 3. Extract from CSD tutorial notebook, run on https://mybinder.org. Via https://losc.ligo.org/tutorials/.

Welcome a disk-shaped flat sheet is wrapped around a sphere. It wrinkles to avoid compression in the longitudinal direction. Image courtesy of [1].

15 https://mybinder.org/
16 https://losc.ligo.org/tutorials/
Underlying Laws

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of 1/4. In collaboration with various SFI colleagues, West found an explanation for this property in the structure of so-called "vital networks," the most obvious examples being the mammalian network of veins and arteries and the fiber bundle structure of plants and trees. Cities also rely on vital networks, such as transportation networks, natural gas and electrical networks, water mains, and sewer lines. Corporations have organization charts and communication networks that are often quite different. All such networks appear fractal in the sense that, by zooming in on successively smaller parts of the whole, one discovers a series of remarkably similar branching diagrams.

West and his coworkers soon concluded that vital networks share three essential characteristics: they are (i) space-filling, in that they reach every extremity of the host body; (ii) have a finite fractal dimensionality; and (iii) account for numerous properties of plant and animal life, including the ability to predict, among other things, the food requirements of animals as they progress from birth to market weight. Growth is accomplished primarily through cell division, which proceeds at a rate roughly proportional to the number of cells in place, and hence to body mass $m(t)$. West concludes that

$$m(t) = m_0 t^{1/4},$$

where $t = 3/4$. The first term on the right represents the metabolic rate, while the second represents cell division. One may deduce species-specific constants $a$ and $b$ from measurements taken in the field and/or laboratory. Solutions are generally S-shaped, rising first slowly, then steeply from a birth weight $m_0$, near 0 before leveling off at the maximum sustainable level determined by setting $d m/d t = 0$. The substitution $m = m_0 a t^{1/4}$ reduces (1) to a linear equivalent.

More remarkably, West has identified dimensionless exponents $\alpha$ and $\gamma$ in terms of which many (possibly all) species share the common growth curve $m(t) = m_0 t^{1/4}$. To justify such a universal claim, he assigns specific colors and shapes to different animal species. And if that can occur once, it can happen many times, as suggested in Figure 2.

Unfortunately, these progress-preserving innovations must keep growing larger and more frequent, meaning that the gaps between the vertical asymptotes of Figure 2 will narrow with the passage of time. This lends credence to the fear expressed by John von Neumann shortly before his death in 1957: mankind seems to be approaching an era of "technological singularity" in which it may become impossible to prolong the era of rapid progress initiated by the Industrial Revolution. (1)

Geoffrey West's Scale is a landmark volume full of interesting ideas and engaging digressions that expand the book with both entertainment and cognitive value. James Case writes from Baltimore, Maryland.
Measuring Areas with a Shopping Cart

One late night in a deserted supermarket, I was waiting in a check-out aisle for a cashier. With no one around and nothing better to do, I began rolling the shopping cart’s front wheel around the outline of a floor tile. The cart ended up rotated after one traversal, as Figure 1 illustrates (for a round “bike” and with a “bike” instead of a shopping cart). It then dawned on me that the angle \( \theta \) by which the cart turns in one cycle (see Figure 1), is proportional to the area \( A \) of the tile, up to a small relative error if the diameter \( d \) of the cart (not necessarily a circle) is small:

\[
A = \frac{\pi d^2}{4},
\]

where \( L \) is the length of the “bike.”

As happens with nearly every observa- tion, someone noticed this before. Holger Prytz (a Danish cavalry officer) proposed the idea of calculating areas more than 100 years ago, and without the advantage of a shopping cart. One can find a beautiful description of this in [2], along with the discovery that the bike’s direction angle changes after a cycle according to the Möbius transformation restricted to a circle, so

\[
z = e^{2\pi i \theta} - a = \frac{z - a}{1 - \overline{a} z},
\]

where \( a \) and \( \theta \) are functional- ions of the front path. The Prytz planimeter, also called the hatchet planimeter, is sketched in Figure 2. The hatchet moves like a rear wheel, not sliding side- ways. The me- ridian is guided around the region’s bound- ary, and the angle \( \theta \) gives the area according to (1). A geometrical explanation of (1) rests on two observations of independent interest.

**Observation 1**

The signed area \( \gamma \) swept by a moving segment (as described in Figure 3) remains unchanged if the longitudinal velocity is altered (and in particular made to vanish). This statement is intuitively plausible since the longitudinal motion has no effect on the rate at which \( RF \) sweeps the area.

\[
\text{Area swept by } RF = \int_0^{2\pi} \gamma dt.
\]

But this area equals \( A = \frac{1}{2} A_{\text{RF}} \) by Observation 2, so that

\[
A = \frac{1}{2} A_{\text{RF}} = \frac{1}{2} \int_0^{2\pi} \gamma dt.
\]

It is not hard to show that \( A_{\text{RF}} = O(\gamma) \); this completes the outline of the proof of (1).

The doubly-swept area contributes zero, leav- ing \( A_{\text{RF}} \) as the net swept area.

2017 SIAM/Analysis of Partial Differential Equations Prize

Scott N. Armstrong (Courant Institute, New York University) and Charles K. Smart (University of Chicago) were awarded the 2017 SIAM Activity Group on Analysis of Partial Differential Equations (SIAG/PADE) Prize for their paper, “Quantitative Stochastic Homogenization of Convex Integral Functionals,” published in Annales Scientifiques de l’École Normale Supérieure in 2016. They received their awards at the 2017 SIAM Conference on Analysis of Partial Differential Equations, held last December in Baltimore, Md., where Armstrong also gave a talk entitled “Quantitative Stochastic Homogenization by Variational Methods.”

The SIAG/PADE Prize is awarded biennially to the author or authors of the most outstanding paper, according to the prize com- mittee, published in a peer-reviewed journal in the three calendar years preceding the award year. The 2017 prize committee states that Armstrong and Smart’s work “obtained outstanding results and developed fun- dumental new techniques that have greatly advanced the field and opened the path to further developments.”

Scott Armstrong is currently an associ- ate professor at New York University’s Courant Institute of Mathematical Sciences. His research lies at the intersection of prob- ability and analysis, with a recent focus on stochastic homogenization of partial dif- ferential equations (PDEs). Charles Smart is an associate professor of mathematics at the University of Chicago. He is particularly interested in the interaction of nonlinear PDEs and probability, in the form of either scaling limits of statistical physics models or homogenization of PDEs with random coefficients.

Why are you excited to be receiving this prize?

We are deeply honored to win this prize and grate- ful to the committee for acknowledging our work in this way. There has been a lot of interesting math- ematics in the last several years on the topic of quantitative stochastic homogenization, and we hope that the prize shines a spotlight not just on our paper but also on the work of our collaborators, Tuomo Kuusi and Jean-Christophe Mourrat, as well as the excellent work of others, such as Antoine Gloria and Felix Otto, who really inspired us.

Can you tell us a bit about the research that won you the prize?

Our research is about the behavior of solutions to certain PDEs, with coefficients that are randomly oscillating on very small length scales. These equations model physical properties (like electrical or thermal conductivity) of com- posite materials. On smaller scales, the solutions behave very erratically since they depend on the equation’s ran- dom oscillations; this is very hard to analyze. Researchers want to be able to rigorously prove that on large mac- roscopic length scales the solutions behave in a much simpler way because all of this randomness averages out in some sense. This phe- nomenon is called “homogeniza- tion,” and the theory has many similarities to problems in statistical physics and probability theory. There has recently been a lot of focus among research- ers on understanding more precisely this homogenization approxima- tion’s ability to describe the real solution. In our paper, we introduced some new ideas for obtaining quantitative bounds on the homogenization error, which arose out of the variational formulation of the equations.

The variational interpretation of the equa- tions gives a rigorous way of implementing a "renormalization" approach to the problem, and in later work our methods subsequently lead to an essentially optimal quantitative theory for this specific model.

What does your research mean to the public?

We hope that our research, and that of others working on similar topics, will yield new mathematical approaches for understanding other equations with random coefficients as well as similar models of physical systems. There is still much to understand at the level of basic research. The math- ematics we have develop- ed also offers a math- ematical foundation for the design of numerical algorithms for computing the macroscopic proper- ties of composite materi- als, which is of practical importance to engineers.

What does what being a SIAM member mean to you?

SIAM plays an indis- pensable role in pro- moting applied mathematics, supporting mathematical research, and allowing us to com- municate our work, keep up-to-date on the latest exciting research, and collaborate with each other.
Reservoir Computing: Harnessing a Universal Dynamical System

By Daniel J. Gauthier

There is great current interest in developing artificial intelligence algorithms for processing massive data sets, often for classification tasks such as recognizing a face in a photograph. But what if our goal is to learn a dynamical system? Relevant applications include forecasting the weather, controlling complex dynamical systems, and finding radio-frequency transmitters to secure the internet of things.

Training a "universal" dynamical system to predict the behavior of a desired system is one approach to this problem that is well-suited for a reservoir computer (RC): a recurrent artificial neural network for processing time-dependent information (see Figure 1). It can operate in many modes, including prediction mode, the task described above. While researchers have studied RCs for well over 20 years [1] and applied them successfully to a variety of tasks [2], there are still many open questions about whether the dynamical systems community may find interesting and be able to address.

An RC is distinguished from traditional feed-forward neural networks by the following qualities:

• The network nodes each have distinct dynamical properties.
• Time delays of signals may occur along the network links.
• The network’s hidden part has recurrent connections.
• The inputs and internal weights are fixed and chosen randomly.
• Only the output weights are adjusted during training.

The last point drastically speeds up the training process.

Mathematically, an RC is described by the set of autonomous, time-delay differential equations given by

\[
\frac{dx}{dt} = -\gamma x + J^\top W_{\text{in}} u(t) + \sum_{k=1}^{N} W_{\text{res}} x_k(t - \tau_k) + \epsilon i(t),
\]

(1)

where \(J\) is the input matrix, \(N\) reservoir nodes \(x_k\), and \(K\) outputs with values \(y_k\). Here, \(\gamma\) are decay constants, \(W_{\text{res}}\) are fixed input (internal) weights, \(\tau_k\) are link time delays, \(\epsilon\) is bias, and \(W_{\text{in}}\) are the output weights whose values are optimized for a particular task. The non-linear function \(f\) is typically sigmoidal, which we can take to the limit of an on-off thresholding (Boolean) function, as is done in traditional Hopfield networks. The reservoir maps the input data streams to a higher dimensional phase space—dimension expansion.

For the prediction task, we are \(W_{\text{in}}\) using a finite-duration “training” data sample so that the resulting output represents the predictions of a long-timescale system. After training, the input signals are disconnected and the outputs are wired to inputs to start the prediction phase.

In general, \(W_{\text{res}}\) is determined by injecting an input training data set \(U\) over a time \(T_{\text{train}}\) and observing the network dynamics \(x\) over this interval. Based on these observations, we modify the weights to minimize the error of the output \(Y\) to the desired output \(Y^\star\), resulting in

\[
W_{\text{res}} = Y^\star X^\top (XX^\top + \alpha I)^{-1},
\]

(2)

where \(\alpha\) is a regularization parameter, \(I\) is the identity matrix, and \(T\) indicates the transpose.

We can solve (2) in a least-squares sense using pseudo-inverse matrix routines that are often included in a variety of computer languages, some of which can take advantage of the matrices’ sparseness. A nonzero value of \(\alpha\) ensures that the norm of \(W_{\text{res}}\) does not become large, which improves the generalizability of the system to different inputs and increases noise tolerance. We can also find a solution to (2) using gradient descent methods, which are helpful when the matrix dimensions are large, and leverage tool-kits from the deep learning community that take advantage of graphical processing units. Use of recursive least-squares is another approach.

An RC can work very well in the prediction task. For example, it is possible to learn the behavior of a dynamical system when the reservoir dynamics is projected to a lower-dimensional phase space before training [3]. We can also learn the attractor with standard training approaches and accurately find Lyapunov exponents from the time series produced by the RC, even for spatial-temporal dynamics [7]. Furthermore, we can utilize the predicted time series as an observer in a control system [4] or for data assimilation of large spatiotemporal systems without use of an underlying model [6]. These results suggest that an RC is a powerful tool for characterizing complex dynamical systems.

While these conclusions are compelling, designing an RC for a particular task is largely a trial-and-error undertaking, and authors tend to present results that work without dwelling on those that fail. The following is an open question: how can we optimize the parameters in (1) and (2) to obtain the most accurate prediction in either the prediction or classification tasks, while simultaneously allowing the RC to function well on data that is similar to the training data set? Early studies focused on the so-called echo state property of the network—where the output should eventually forget the input—and the consistency property, where outputs from identical trials should be similar over some period. These conditions were initially assumed to be guaranteed when the spectral radius of \(W_{\text{res}}\) is less than one (for the case when \(\alpha = 0\)). However, this scenario ignores the input dynamics and is a mostly a statement of the stability of \(X = 0\). Recent work is beginning to address this shortcoming for the case of a single input channel, demonstrating that there must be a single entire output solution given the input [5].

While a base of past research exists, many questions that demand quantitative model-free answers remain. For example, how large must \(\alpha\) be to achieve a desired error rate? How should we adjust \(\gamma\), relative to the timescales of the dynamical system? Why do sparsely-connected reservoirs often perform best?

At the 2017 SIAM Conference on Applications of Dynamical Systems, held in Snowbird, Utah, last May, Edward Ott and I organized a minisymposium on RCs to discuss these and other problems. Ott showed that RCs can learn the “climate” of a dynamical system and accurately forecast spatiotemporal chaos in a scalable manner. Roger Brockett indicated that dense network connections might give rise to partial or full synchronization of the reservoir nodes, thus diminishing the diversity of waveforms that an RC can learn. Brian Hunt suggested that an RC must synchronize to the input data in a generalized sense when used for the prediction task. Finally, I discussed a hardware-based RC capable of predicting at a rate exceeding tens of MHz. In summary, RCs can serve as a universal dynamical system capable of learning the dynamics of other systems. This may prove advantageous when obtaining data for the learned dynamical system is expensive or difficult, for example. While the field is progressing rapidly, there are still substantial openings for others to join the effort.

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References


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The 2018 SIAM Annual Meeting is co-located with the 2018 SIAM Conference on Mathematical Aspects of Materials Science. My invited talk, which is part of both meetings, will develop the aforementioned topics, focused on recent examples in which the identification of energy scaling laws has produced some interesting surprises.

References


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