



Mathematical Software

Is It Mathematics or Is It Software?

Lisa R. Goldberg

Note: The opinions expressed here are not necessarily those of Notices. Responses on the Notices webpage are invited.

Computers can empower mathematicians to envision and to prove theorems beyond natural limitations. At the same time, computers can facilitate misdirection and error on a grand scale. Working on software development is, in effect, engaging in an interesting genre of mathematical thinking. Since we are in an age where significant progress has been achieved on both practical and intellectual levels by such thinking, the development of mathematical software is genuinely part of mathematics. That is, the conceptual breakthroughs in software development should find a home in the academic mathematical community.

The Mandelbrot Set

In the early 1900s French mathematicians Pierre Fatou and Gaston Julia laid the groundwork for the dynamics of rational maps of one complex variable. They found that iteration of a nonlinear rational map splits the plane into a pair of invariant sets with distinct profiles. The *Fatou set* is a region of orderly behavior, where nearby points have similar trajectories. For example, they may tend toward an attracting periodic point. The complementary *Julia set* is a region of chaos, where trajectories of nearby points can differ in ways that are impossible to predict. The dynamics of rational maps was an active area of research at the time of Fatou and Julia. However, the subject faded into obscurity and lay dormant until it was reinvigorated by software half a century later.

Polynomials are the most approachable rational maps, and quadratic polynomials of the form

$$\phi_c(z) = z^2 + c$$

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exhibit a dichotomy. The Julia set of ϕ_c is either connected or totally disconnected, depending on whether the trajectory of 0 is bounded. In 1978, mathematicians Robert Brooks and Peter Matelski exploited this property to depict the set of c 's for which the Julia set of ϕ_c is connected.

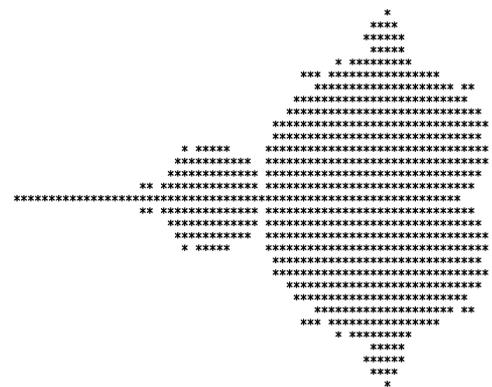


Figure 1. Original image of the Mandelbrot set, plotted by Robert Brooks and Peter Matelski in 1978.

The odd image in Figure 1 caught the imagination of mathematicians, who generated beautiful and suggestive portrayals of what has become known as the *Mandelbrot set*. The more detailed image in Figure 2 hints at its complexity.

In 1975, three years before Brooks and Matelski drew the Mandelbrot set, the physicist Mitchell Feigenbaum was studying the dynamical behavior of quadratic polynomials on the real line. For c between 0 and $-3/4$, the map ϕ_c has a single attracting fixed point. At $c = -3/4$, the fixed attractor bifurcates into a period two attractor, and period doubling of the attractor continues at a decreasing set of parameter values that tend to a chaos parameter. Using an HP-65 calculator, Feigenbaum observed that successive ratios of intervals between period-doubling parameters converged to what has become known as the Feigenbaum constant, approximately 4.6692016148. The Feigenbaum constant was discovered independently by Pierre Couillet and Charles Tresser. The parameter space for quadratic polynomials on the line embeds in the Mandelbrot set,

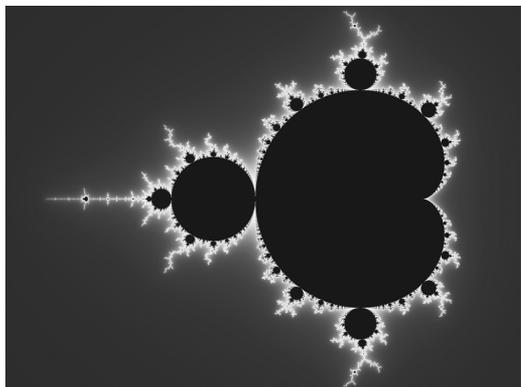


Figure 2. A more detailed image of the Mandelbrot set hints at its complexity.

and Feigenbaum's chaos parameter is at the tail end of a shrinking sequence of balls attached to the central cardioid, as in Figure 3.

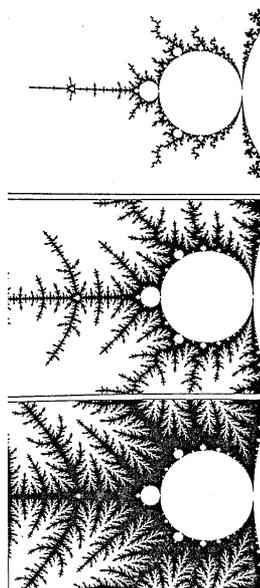


Figure 3. Successive blowups of the neighborhood of the chaos point identified by Feigenbaum, Coulet, and Tresser.

It is impossible to decouple the evolution of the theory of rational maps from the development of the mathematical software that illuminated the theory. As Tony Phillips and I wrote in 1993 about the work of Jack Milnor on the occasion of his sixtieth birthday:

Of special note is an unconventional article entitled "Self-similarity and hairiness in the Mandelbrot set," where he presents some of his numerical experiments in holomorphic dynamics and uses them as evidence for a set of conjectures. Milnor, usually meticulous about complete mathematical arguments, here has no theorems and no proofs. Rather, he brings his mathematical

strength and imagination to bear on every detail of the design and implementation of his experiments. The resulting data are so compelling as to suggest not only what the conjectures should say, but how they can be proved.

Analogs of Feigenbaum's period-doubling descent to chaos are found throughout the Mandelbrot set. Milnor's conjectures in his 1989 paper include an assertion that the Mandelbrot set is self-similar in the neighborhood

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of *chaos parameters*, limits of period-doubling parameters. Scale vanishingly small neighborhoods of a chaos parameter by powers of the Feigenbaum constant and you see the same image over and over again. Conjectures from Milnor's article were proved without the direct aid of computers by Mikhail Lyubich in 1999.

Feigenbaum discovered a universal principle with a calculator. Brooks and Matelski stumbled on an odd image with a primitive computer program. Mandelbrot saw the possibilities in that image, which bears his name. Milnor designed and implemented mathematical software to formulate conjectures related to the Mandelbrot set. At each step, computers augmented human ability, allowing us to attain new advances and insights.

Flawed Software Leads to Flawed Science

Greater demand for mathematical software has led to specialization and a growing gap between development and application. This extends our reach, but it is risky.

In 2010 economists Carmen Reinhart of the University of Maryland and Kenneth Rogoff of Harvard University released a paper entitled "Growth in a time of debt," which linked higher debt-to-GDP ratios with lower growth. This influential article gave support to policymakers who wanted to restrain borrowing at a time when governments were struggling to address the severe consequences of the 2008 financial crisis. But the analysis in the article was wrong. Among the impactful errors made by the authors was a code bug that omitted data about Australia, Austria, Belgium, Canada, and Denmark from estimates. That bug accounted for roughly 30 percent of the reported difference in growth rates in lower and higher debt-to-GDP countries.

Code bugs are not the only flaws in software. In a 2016 empirical study, biomedical scientists Anders Eklund, Thomas Nichols, and Hans Knutsson discuss the impact of an erroneous statistical assumption in software for interpreting functional magnetic resonance imaging (fMRI). The implications are profound, since fMRI is used

by brain surgeons to assess the riskiness of invasive treatment and to map damage from tumors and strokes. As Eklund, Nichols, and Knutsson emphasize in their article:

Functional MRI (fMRI) is 25 years old, yet surprisingly its most common statistical methods have not been validated using real data...In theory, we should find 5 percent false positives (for a significance threshold of 5 percent), but instead we found that the most common software packages for fMRI analysis can result in false-positive rates of up to 70 percent. These results question the validity of some 40,000 fMRI studies and may have a large impact on the interpretation of neuroimaging results.

The problem, according to the authors, is “spatial autocorrelation functions that do not follow the assumed Gaussian shape.” The “Gaussian shape” is embedded in standard packages such as Excel, and it is the default for determining statistical significance throughout the social sciences, whether or not it is an appropriate description of the data.

In a 2015 article, Bob Anderson, Stephen Bianchi, and I describe a stunning false positive in a 2006 article by financial economists Andrew Ang, Robert Hodrick, Yuhang Xing, and Xiaoyan Zhang. Oblivious to a 26-sigma outlier, the authors used the “Gaussian shape” to infer statistical significance of a financial risk factor. Their article has 2,222 citations on Google Scholar, while our article detailing the erroneous inference has 4 citations.

The damage done by erroneous inference based on an assumed “Gaussian shape” is only beginning to be understood.

Commercial versus Open Source

The UCLA mathematics department software page lists five packages that cover a wide range of applications. The first three packages—Maple, Mathematica, and Matlab—are commercial, while the last two, Octave and SageMath, are open source. These packages are essential elements of educational programs, and they facilitate quantitative research in academia and industry.

The benefits of commercial and open source software are complementary. Commercial providers have incentives to offer easy-to-use interfaces, novice-safe routines, and customer service—in other words, to serve a broad and heterogeneous group of users. The motivation for open source providers is summarized by the GNU Manifesto: freedom to run a program for any purpose, freedom to study the mechanics of the program and modify it, freedom to redistribute copies, and freedom to improve and change modified versions for public use. This was written in 1983 by Richard Stallman as part of a request for support for MIT’s GNU Project, the free software movement. GNU includes Octave, and GNU packages such as R are part of SageMath.

Launched in 2005 by number theorist and software developer William Stein, SageMath is true to the GNU Manifesto. It has benefitted from more than 500 unpaid

contributors and serves, by a conservative estimate, more than 50,000 active users. SageMath performs standard mathematical tasks such as optimization, statistical simulation, and matrix algebra. It also performs more exotic tasks, such as the calculation of the modular degree of an elliptic curve, and its web-based computing environment, SageMathCloud, includes \TeX and courseware. Despite its breadth and popularity, SageMath has not found adequate funding in the academic mathematics community, and Stein is going commercial.

Reproducibility

Reproducibility is actually the heart of science.

—Eric Lander

A *Pythagorean triple-free split* of $S \subset \mathbb{N}$ is a decomposition of S into a disjoint pair of subsets, neither of which contains a complete Pythagorean triple. In the 1980s Ron Graham offered a \$100 prize for a solution to the Boolean Pythagorean Triples problem: Is there is a Pythagorean triple-free split of the natural numbers?

In May 2016 computer scientists Martin J. H. Huele, Oliver Kullman, and Victor W. Marek posted an article on arXiv arguing that there is a Pythagorean triple-free split for $S = \{1, 2, \dots, N\}$ so long as $N < 7284$, but no such split exists when $N = 7285$. This is a recent addition to the library of computer-assisted results, which includes the four color map theorem and the proof of the Kepler conjecture. Graham awarded the \$100 prize to the authors for their publicly-available-yet-inscrutable 200-terabyte proof. Validation by the academic community may follow more closely the practices of science rather than mathematics. Can independent teams of researchers with different computers and different software replicate the results?

The Reproducibility Project was an attempt by a collection of 270 scientists to replicate one hundred studies published in high-ranking psychology journals in 2008. They found that only one-third to one-half of the studies could be replicated. This is consistent with the prediction of Stanford Medical School professor John Ioannidis, who argued in a 2005 article that most published research findings are false.

Best practices for reproducible research have been developed by the Reproducibility and Open Science Working Group, which is based at New York University, UC Berkeley, and University of Washington. Their mission is to support “software tools and practices that support the sharing, preservation, provenance, and reproducibility of data, software, and scientific workflows.” Reproducible science is, of course, a laudable goal, but it will require substantial discipline on the part of the academic community and perhaps a modification of its incentive structure.

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Diaspora

It is a tradition at the UC Berkeley mathematics department graduation to announce students' plans for the future as they receive their diplomas. I listened with pleasure to the graduates' hopeful next steps. Some students were enrolled in PhD programs or professional schools, others were planning to travel, still others were joining startups or well-established corporations. There were many aspiring software developers, and I thought to myself that they are not leaving mathematics, but rather, extending its reach.

Credits

Figure 1 is in the Public Domain.

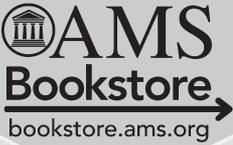
Figure 2 was created by Wolfgang Beyer with the program Ultra Fractal 3. Used under the terms of the Creative Commons License.

Figure 3 was originally published in "Self-similarity and hairiness in the Mandelbrot set," *Computers in Geometry and Topology*, M. C. Tangora, editor, Marcel Dekker, New York, Basel, 1989, pp. 211–257. Reprinted by permission of Taylor & Francis. (www.tandfonline.com).

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