THE COMPUTER AS CRUCIBLE

AN INTRODUCTION TO EXPERIMENTAL MATHEMATICS

JONATHAN BORWEIN • KEITH DEVLIN

The Computer as Crucible

The Computer as Crucible

An Introduction to Experimental Mathematics

Jonathan Borwein
Keith Devlin
with illustrations by Karl H. Hofmann

A K Peters, Ltd.
Natick, Massachusetts

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742

Version Date: 20150213

International Standard Book Number-13: 978-1-4398-7691-6 (eBook - PDF)

Visit the Taylor & Francis Web site at
http://www.taylorandfrancis.com

and the CRC Press Web site at
http://www.crcpress.com

For *Jakob Joseph*, age two,
and all others who will experience
much more powerful mathematical crucibles

Contents

Preface

Our aim in writing this book was to provide a short, readable account of experimental mathematics. (Chapter 1 begins with an explanation of what the term "experimental mathematics" means.) It is not intended as a textbook to accompany a course (though good instructors could surely use it that way). In particular, we do not aim for comprehensive coverage of the field; rather, we pick and choose topics and examples to give the reader a good sense of the current state of play in the rapidly growing new field of experimental mathematics. Also, there are no large exercise sets. We do end each chapter with a brief section called "Explorations," in which we give some follow-up examples and suggest one or two things the reader might like to try. There is no need to work on any of those explorations to proceed through the book, but we feel that trying one or two of them is likely to increase your feeling for the subject. Answers to those explorations can be found in the "Answers and Reflections" chapter near the end of the book.

This book was the idea of our good friend and publisher (plus mathematics PhD) Klaus Peters of A K Peters, Ltd. It grew out of a series of three books that one of us (Borwein) coauthored on experimental mathematics, all published by A K Peters: Jonathan Borwein and David Bailey's *Mathematics by Experiment* (2004); Jonathan Borwein, David Bailey, and Roland Girgensohn's *Experimentation in Mathematics* (2004); and David Bailey, Jonathan Borwein, Neil J. Calkin, Roland Girgensohn, D. Russell Luke, and Victor H. Moll's *Experimental Mathematics in Action* (2007).

We both found this an intriguing collaboration. Borwein, with a background in analysis and optimization, has been advocating and working in the new field of experimental mathematics for much of his career. This pursuit was considerably enhanced in 1993 when he was able to open the Centre for Experimental and Constructive Mathematics at Simon Fraser University, which he directed for a decade. (Many of the results presented here are due to Borwein, most often in collaboration with others, particularly Bailey.) Devlin, having focused on mathematical logic and set theory for the first half of his career, has spent much of the past twenty years looking at the emerging new field known as mathematical cognition, which tries to understand how the human brain does mathematics, how it acquires mathematical ability in the first place, and how mathematical thinking combines with other forms of reasoning, including machine computation. In working together on this book, written to explain to those not in the field what experimental mathematics is and how it is done, Borwein was on the inside looking out, and Devlin was on the outside looking in. We saw reassuringly similar scenes.

Experimental mathematics is fairly new. It is a way of doing mathematics that has been made possible by fast, powerful, and easy-to-use computers, by networks, and by databases.

The use of computers in mathematics *for its own sake* is a recent phenomenon—much more recent than the computer itself, in fact. (This surprises some outsiders, who assume, incorrectly, that mathematicians led the computer revolution. To be sure, mathematicians invented computers, but then they left it to others to develop them, with very few mathematicians actually using them until relatively recently.)

In fact, in the late 1980s, the American Mathematical Society, noting that mathematicians seemed to be lagging behind the other sciences in seeing the potential offered by computers, made a deliberate effort to make the mathematical community more aware of the possibilities presented by the new technology. In 1998, their flagship newsletter, the *Notices of the American Mathematical Society*, introduced a "Computers and Mathematics" section, edited originally by the late Jon Barwise, then (from October 1992 through December 1994) by Devlin. Devlin's interest in how the use of computers can change mathematical practice was part of his growing fascination with mathematical cognition. Correspondingly, Borwein's experience led to a growing interest in mathematical visualization and mathematical aesthetics.

A typical edition of the "Computers and Mathematics" section began with a commissioned feature article, followed by reviews of new mathematical software systems. Here is how Devlin opened his first "Computers and Mathematics" section: "Experimental mathematics is the theme of this month's feature article, written by the Canadian mathematical brothers Jonathan and Peter Borwein."

With this book, the circle is complete!

The "Computers and Mathematics" section was dropped in January 1995, when the use of computers in the mathematical community was thought to have developed sufficiently far that separate treatment in the

Notices was no longer necessary. As this short book should make abundantly clear, things have come a long way since then.

Both authors want to thank Klaus Peters for coming up with the idea for this book, and for his continued encouragement and patience over the unexpectedly long time it took us to mesh our sometimes insanely busy schedules sufficiently to make his vision a reality.

Jonathan Borwein
Keith Devlin

March 2008

What do I see here?

Chapter 1

What Is Experimental Mathematics?

I know it when I see it.
—Potter Stewart (1915–1985)

United States Supreme Court justice Potter Stewart famously observed in 1964 that, although he was unable to provide a precise definition of pornography, "I know it when I see it." We would say the same is true for experimental mathematics. Nevertheless, we realize that we owe our readers at least an approximate initial definition (of experimental mathematics, that is; you're on your own for pornography) to get started with, and here it is.

Experimental mathematics is the use of a computer to run computations—sometimes no more than trial-and-error tests—to look for patterns, to identify particular numbers and sequences, to gather evidence in support of specific mathematical assertions that may themselves arise by computational means, including search. Like contemporary chemists—and before them the alchemists of old—who mix various substances together in a crucible and heat them to a high temperature to see what happens, today's experimental mathematician puts a hopefully potent mix of numbers, formulas, and algorithms into a computer in the hope that something of interest emerges.

Had the ancient Greeks (and the other early civilizations who started the mathematics bandwagon) had access to computers, it is likely that the word "experimental" in the phrase "experimental mathematics" would be superfluous; the kinds of activities or processes that make a particular mathematical activity "experimental" would be viewed simply as *mathematics*. We say this with some confidence because if you remove from our initial definition the requirement that a computer be used, what would be

left accurately describes what most, if not all, professional mathematicians spend much of their time doing, and always have done!

Many readers, who studied mathematics at high school or university but did not go on to be professional mathematicians, will find that last remark surprising. For that is not the (carefully crafted) image of mathematics they were presented with. But take a look at the private notebooks of practically any of the mathematical greats and you will find page after page of trial-and-error experimentation (symbolic or numeric), exploratory calculations, guesses formulated, hypotheses examined (in mathematics, a “hypothesis” is a guess that doesn’t immediately fall flat on its face), etc.

The reason this view of mathematics is not common is that you have to look at the private, *unpublished* (during their career) work of the greats in order to find this stuff (by the bucketful). What you will discover in their *published* work are precise statements of true facts, established by logical proofs that are based upon axioms (which may be, but more often are not, stated in the work).

Because mathematics is almost universally regarded, and commonly portrayed, as the search for pure, eternal (mathematical) truth, it is easy to understand how the published work of the greats could come to be regarded as constitutive of what mathematics actually *is*. But to make such an identification is to overlook that key phrase "the search for." Mathematics is not, and never has been, merely the end product of the search; the process of discovery is, and always has been, an integral part of the subject. As the great German mathematician Carl Friedrich Gauss wrote to his colleague Janos Bolyai in 1808, "It is not knowledge, but the act of learning, not possession but the act of getting there, which grants the greatest enjoyment."[1]

In fact, Gauss was very clearly an "experimental mathematician" of the first order. For example, in 1849 he recounted his analysis of the density of prime numbers [Goldstein 73]:

> I pondered this problem as a boy, in 1792 or 1793, and found that the density of primes around t is $1/\log t$, so that the number of primes up to a given bound x is approximately
>
> $$\int_2^x dt/\log t.$$

Formal proof that Gauss's approximation is asymptotically correct, which is now known as the Prime Number Theorem, did not come until 1896, more than 100 years after the young genius made his experimental discovery.

To give just one further example of Gauss's "experimental" work, we learn from his diary that, one day in 1799, while examining tables of integrals provided originally by James Stirling, he noticed that the reciprocal of the integral

$$\frac{2}{\pi}\int_0^1 \frac{dt}{\sqrt{1-t^4}}$$

agreed numerically with the limit of the rapidly convergent arithmetic-geometric mean iteration (AGM):

$$a_0 = 1, \quad b_0 = \sqrt{2};$$

$$a_{n+1} = \frac{a_n + b_n}{2}, \quad b_{n+1} = \sqrt{a_n b_n}.$$

[1]The complete quote is: "It is not knowledge, but the act of learning, not possession but the act of getting there, which grants the greatest enjoyment. When I have clarified and exhausted a subject, then I turn away from it, in order to go into darkness again; the never-satisfied man is so strange if he has completed a structure, then it is not in order to dwell in it peacefully, but in order to begin another. I imagine the world conqueror must feel thus, who, after one kingdom is scarcely conquered, stretches out his arms for others."

The sequences (a_n) and (b_n) have the common limit

$$1.1981402347355922074\ldots.$$

Based on this purely computational observation (which he made to 11 places), Gauss conjectured and subsequently proved that the integral is indeed equal to the common limit of the two sequences. It was a remarkable result, of which he wrote in his diary, "[the result] will surely open up a whole new field of analysis." He was right. It led to the entire vista of nineteenth-century elliptic and modular function theory.

For most of the history of mathematics, the confusion of the activity of mathematics with its final product was understandable: after all, both activities were done by the same individual, using what to an outside observer were essentially the same activities—staring at a sheet of paper, thinking hard, and scribbling on that paper.[2] But as soon as mathematicians started using computers to carry out the exploratory work, the distinction became obvious, especially when the mathematician simply hit the ENTER key to initiate the experimental work, and then went out to eat while the computer did its thing. In some cases, the output that awaited the mathematician on his or her return was a new "result" that no one had hitherto suspected and might have no inkling how to prove.

The scare quotes around the word "result" in that last paragraph are to acknowledge that the adoption of experimental methods does not necessarily change the notion of mathematical truth, nor the basic premise that the only way a mathematical statement can be certified as correct is when a formal proof has been found. Whenever a relationship has been obtained using an experimental approach—and in this book we will give many specific examples—finding a formal proof remains an important and legitimate goal, although not the only goal.

What makes experimental mathematics different (as an enterprise) from the classical conception and practice of mathematics is that the experimental process is regarded not as a precursor to a proof, to be relegated to private notebooks and perhaps studied for historical purposes only after a proof has been obtained. Rather, experimentation is viewed as a signifi-

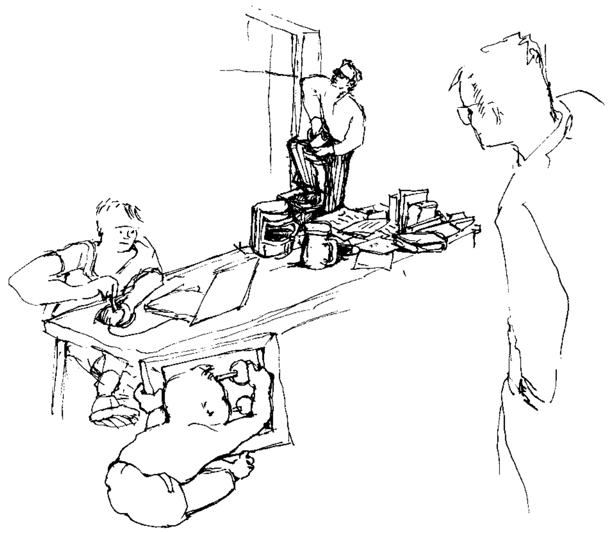
[2]The confusion would have been harmless but for one significant negative consequence: it scared off many a young potential mathematician, who, on being unable instantaneously to come up with the solution to a problem or the proof of an assertion, would erroneously conclude that they simply did not have a mathematical brain.

cant part of mathematics in its own right, to be published, to be considered by others, and (of particular importance) *to contribute to our overall mathematical knowledge*. In particular, this gives an epistemological status to assertions that, while supported by a considerable body of experimental results, have not yet been formally proved, and in some cases may never be proved. (As we shall see, it may also happen that an experimental process itself yields a formal proof. For example, if a computation determines that a certain parameter p, known to be an integer, lies between 2.5 and 3.784, that amounts to a rigorous proof that $p = 3$.)

When experimental methods (using computers) began to creep into mathematical practice in the 1970s, some mathematicians cried foul, saying that such processes should not be viewed as genuine mathematics—that the one true goal should be formal proof. Oddly enough, such a reaction would not have occurred a century or more earlier, when the likes of Fermat, Gauss, Euler, and Riemann spent many hours of their lives carrying out (*mental*) calculations in order to ascertain "possible truths" (many but not all of which they subsequently went on to prove). The ascendancy of the notion of proof as the sole goal of mathematics came about in the late nineteenth and early twentieth centuries, when attempts to understand the infinitesimal calculus led to a realization that the intuitive concepts of such basic concepts as function, continuity, and differentiability were highly problematic, in some cases leading to seeming contradictions. Faced with the uncomfortable reality that their intuitions could be inadequate or just plain misleading, mathematicians began to insist that value judgments were hitherto to be banished to off-duty chat in the mathematics common room and nothing would be accepted as legitimate until it had been formally proved.

This view of mathematics was the dominant one when both your present authors were in the process of entering the profession. The only way open to us to secure a university position and advance in the profession was to *prove* theorems. As the famous Hungarian mathematician Paul Erdős (1913–1996) is often quoted as saying, "a mathematician is a machine for turning coffee into theorems."[3]

[3] A more accurate rendition is: "Renyi would become one of Erdős's most important collaborators. … Their long collaborative sessions were often fueled by endless cups of strong coffee. Caffeine is the drug of choice for most of the world's mathematicians and coffee is the preferred delivery system. Renyi, undoubtedly wired on espresso, summed this up in a



As it happened, neither author fully bought into this view. Borwein adopted computational, experimental methods early in his career, using computers to help formulate conjectures and gather evidence in favor of them, while Devlin specialized in logic, in which the notion of proof is itself put under the microscope, and results are obtained (and published) to the effect that a certain statement, while true, is demonstrably not provable—a possibility that was first discovered by the Austrian logician Kurt Gödel in 1931.

What swung the pendulum back toward (openly) including experimental methods, we suggest, was in part pragmatic and part philosophical. (Note that word "including." The *inclusion* of experimental processes in no way eliminates proofs. For instance, no matter how many zeroes

famous remark almost always attributed to Erdős: *'A mathematician is a machine for turning coffee into theorems.'* ... Turan, after scornfully drinking a cup of American coffee, invented the corollary: *'Weak coffee is only fit for lemmas'*" [Schecter 98, p. 155].

of the Riemann zeta function are computed and found to have real part equal to 1/2, the mathematical community is not going to proclaim that the Riemann hypothesis—that all zeroes have this form—is true.[4])

The pragmatic factor behind the acknowledgment of experimental techniques was the growth in the sheer *power* of computers to search for patterns and to amass vast amounts of information in support of a hypothesis.

At the same time that the increasing availability of ever cheaper, faster, and more powerful computers proved irresistible for some mathematicians, there was a significant, though gradual, shift in the way mathematicians viewed their discipline. The Platonistic philosophy that abstract mathematical objects have a definite existence in some realm outside of humankind, with the task of the mathematician being to uncover or discover eternal, immutable truths about those objects, gave way to an acceptance that the subject is the product of humankind, the result of a particular kind of human thinking.

In passing, let us mention that the ancient-sounding term "Platonistic," for a long-standing and predominant philosophy of working mathematicians, is fairly recent. It was coined in the 1930s, a period in which Gödel's results made mathematical philosophers and logicians think very hard about the nature of mathematics. Mathematicians largely ignored the matter as of concern only to philosophers. In a similar vein, the linguist Steve Pinker recently wrote: "I don't think bio-chemists are going to be the least bit interested in what philosophers think about genes." This led biologist Steve Jones to retort: "As I've said in the past, philosophy is to science as pornography is to sex: It's cheaper, easier, and some people prefer it."[5]

It would be a mistake to view the Platonist and the product-of-the-human-mind views of mathematics as an exclusive either-or choice. A characteristic feature of the particular form of thinking we call mathematics is that it *can be thought of* in Platonistic terms—indeed most mathematicians report that such is how it appears and feels when they are actually doing mathematics.

[4]Opinions differ as to whether, or to what degree, the computational verification of billions of cases provides meaningful information as to how likely the hypothesis is to be true. We'll come back to this example shortly.

[5]This exchange can be found in *The Scientist*, June 20th, 2005.

The shift from Platonism to viewing mathematics as just another kind of human thinking brought the discipline much closer to the natural sciences, where the object is not to establish "truth" in some absolute sense, but to analyze, to formulate hypotheses, and to obtain evidence that either supports or negates a particular hypothesis.

In fact, as the Hungarian philosopher Imre Lakatos made clear in his 1976 book *Proofs and Refutations*, published two years after his death, the distinction between mathematics and natural science—as practiced—was always more apparent than real, resulting from the fashion among mathematicians to suppress the exploratory work that generally precedes formal proof.

By the mid-1990s, it was becoming common to "define" mathematics as a science—"the science of patterns" (an acceptance acknowledged and reinforced by Devlin's 1994 book *Mathematics: The Science of Patterns*).

The final nail in the coffin of what we shall call "hard-core Platonism" was driven in by the emergence of computer proofs, the first really major example being the 1976 proof of the famous Four Color Theorem, a statement that to this day is accepted as a theorem solely on the basis of an argument (actually, today at least two different such arguments) of which a significant portion is of necessity carried out by a computer.

The degree to which mathematics has come to resemble the natural sciences can be illustrated using the Riemann hypothesis, which we mentioned earlier. To date, the hypothesis has been verified computationally for the *ten trillion* zeroes closest to the origin. But every mathematician will agree that this does not amount to a conclusive proof. Now suppose that, next week, a mathematician posts on the Internet a five-hundred page argument that she or he claims is a proof of the hypothesis. The argument is very dense and contains several new and very deep ideas. Several years go by, during which many mathematicians around the world pore over the proof in every detail, and although they discover (and continue to discover) errors, in each case they or someone else (including the original author) is able to find a correction. At what point does the mathematical community as a whole declare that the hypothesis has indeed been proved? And even then, which do you find more convincing, the fact that there is an argument for which none of the hundred or so errors found so far have proved to be fatal, or the fact that the hypothesis has been verified computationally (and, we shall assume, *with total certainty*) for 10

Plato: Look, Ari, up there are arbitrarily long arithmetic sequences in the set of primes – and will be there when the sun has engulfed the earth!

Aristoteles: Listen, old man, the computer has driven the final nail into the coffin of your "ideas." Down here is where the action is as long as we and IT are here.

trillion cases? Different mathematicians will give differing answers to this question, but their responses are mere *opinions*.

In one fairly recent case, the editors of the *Annals of Mathematics* decided to publish a proof of a certain result with the disclaimer that after a committee of experts had examined the proof in great details for four years, the most positive conclusion they had been able to arrive at was that they were "99% certain" the argument was correct, but could not be absolutely sure. After other leading mathematicians intervened, the journal editors relented, and the paper was published without the disclaimer, but the point had been established: the mathematical world had changed.

The problematic proof was Thomas Hales's solution of the Kepler sphere packing problem [Hales 05]. It actually involved some computational reasoning, but the principle was established: given sufficient complexity, no human being can ever be certain an argument is correct, nor even a group of world experts. Hales's method ultimately relied on using a linear programming package that certainly gives correct answers but was never intended to certify them.

With a substantial number of mathematicians these days accepting the use of computational and experimental methods, mathematics has indeed grown to resemble much more the natural sciences. Some would argue that it simply *is* a natural science. If so, it does however remain, and we believe ardently will always remain, the most secure and precise of the sciences. The physicist or the chemist must rely ultimately on observation, measurement, and experiment to determine what is to be accepted as "true," and there is always the possibility of a more accurate (or different) observation, a more precise (or different) measurement, or a new experiment (that modifies or overturns the previously accepted "truths"). The mathematician, however, has that bedrock notion of proof as the final arbitrator. Yes, that method is not (in practice) perfect, particularly when long and complicated proofs are involved, but it provides a degree of certainty that no natural science can come close to. (Actually, we should perhaps take a small step backward here. If by "come close to" you mean an agreement between theory and observation to ten or more decimal places of accuracy, then modern physics has indeed achieved such certainty on some occasions.)

So what kinds of things does an experimental mathematician do? More precisely, and we hope that by now our reader appreciates the reason for this caveat, what kinds of activity does a *mathematician* do that classify, or can be classified, as "experimental mathematics"? Here are some that we will describe in the pages that follow:

1. symbolic computation using a computer algebra system such as Mathematica or Maple,

2. data visualization methods,

3. integer-relation methods, such as the PSLQ algorithm (see later),
4. high-precision integer and floating-point arithmetic,
5. high-precision numerical evaluation of integrals and summation of infinite series,
6. use of the Wilf-Zeilberger algorithm for proving summation identities (we're not doing that one),
7. iterative approximations to continuous functions (ditto),
8. identification of functions based on graph characteristics.

We should point out that our brief account in no way sets out to provide a comprehensive coverage of contemporary experimental mathematics. Rather, we focus on a particular slice through the field, by way of providing illustration of this powerful, and growing, new *approach* to mathematical discovery that the computer has made possible. (Though we should repeat our earlier observation that in days past, many of the greatest mathematicians spent many hours in "experimental pursuits," doing masses of computations with no aid other than a pen and paper and the power of their own intellect—or sometimes that of an assistant or two.)[6]

For the most part, our slice comprises (bits of) experimental real analysis and experimental analytic number theory, some of the former coming from problems in modern physics. In the final chapter (Chapter 11), we will provide a very brief survey of the use of experimental methods in some other parts of mathematics.

Explorations

One of the tantalizing things about computer experimentation is to learn how to distinguish when you might learn something by experimenting and when "messing about" is a waste of time. Ideally, you should run every experiment like a rigorous biology experiment with a null hypothesis,

[6]Until the second half of the twentieth century, the English word "computer" was used to refer to a human being, not a machine.