

SECOND EDITION

Mathematics by Experiment

PLAUSIBLE REASONING IN THE 21ST CENTURY

Jonathan Borwein
David Bailey

Mathematics by Experiment
Plausible Reasoning in the 21st Century
Second Edition

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David Bailey



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Preface

[I]ntuition comes to us much earlier and with much less outside influence than formal arguments which we cannot really understand unless we have reached a relatively high level of logical experience and sophistication. . . . In the first place, the beginner must be convinced that proofs deserve to be studied, that they have a purpose, that they are interesting.

George Polya, *Mathematical Discovery: On Understanding, Learning and Teaching Problem Solving*, 1968

The authors first met in 1985, when Bailey used the Borwein quartic algorithm for π as part of a suite of tests on the new Cray-2 then being installed at the NASA Ames Research Center in California. As our collaboration has grown over the past 18 years, we have become more and more convinced of the power of experimental techniques in mathematics. When we started our collaboration, relatively few mathematicians employed computations in serious research work. In fact, there appeared to be a widespread view in the field that “real mathematicians don’t compute.” In the ensuing years, computer hardware has skyrocketed in power and plummeted in cost, thanks to the remarkable phenomenon of Moore’s Law. In addition, numerous powerful mathematical software products, both commercial and noncommercial, have become available. But just importantly, a new generation of mathematicians is eager to use these tools, and consequently numerous new results are being discovered.

The experimental methodology described in this book, as well as in the second volume of this work, *Experimentation in Mathematics: Computational Paths to Discovery* [72], provides a compelling way to generate understanding and insight; to generate and confirm or confront conjectures; and generally to make mathematics more tangible, lively and fun for both the professional researcher and the novice. Furthermore, the experimental approach helps broaden the interdisciplinary nature of mathematical research: a chemist, physicist, engineer, and a mathematician may not understand each others’ motivation or technical language, but they often

share an underlying computational approach, usually to the benefit of all parties involved.

Our views have been expressed well by Epstein and Levy in a 1995 article on experiment and proof [136].

The English word “prove”—as its Old French and Latin ancestors—has two basic meanings: to try or test, and to establish beyond doubt. The first meaning is largely archaic, though it survives in technical expressions (printer’s proofs) and adages (the exception proves the rule, the proof of the pudding). That these two meanings could have coexisted for so long may seem strange to us mathematicians today, accustomed as we are to thinking of “proof” as an unambiguous term. But it is in fact quite natural, because the most common way to establish something in everyday life is to examine it, test it, probe it, experiment with it.

As it turns out, much the same is true in mathematics as well. Most mathematicians spend a lot of time thinking about and analyzing particular examples. This motivates future development of theory and gives one a deeper understanding of existing theory. Gauss declared, and his notebooks attest to it, that his way of arriving at mathematical truths was “through systematic experimentation.” It is probably the case that most significant advances in mathematics have arisen from experimentation with examples. For instance, the theory of dynamical systems arose from observations made on the stars and planets and, more generally, from the study of physically motivated differential equations. A nice modern example is the discovery of the tree structure of certain Julia sets by Douady and Hubbard: this was first observed by looking at pictures produced by computers and was then proved by formal arguments.

Our goal in these books is to present a variety of *accessible* examples of modern mathematics where intelligent computing plays a significant role (along with a few examples showing the limitations of computing). We have concentrated primarily on examples from analysis and number theory, as this is where we have the most experience, but there are numerous excursions into other areas of mathematics as well (see the Table of Contents). For the most part, we have contented ourselves with outlining reasons and exploring phenomena, leaving a more detailed investigation to the reader. There is, however, a substantial amount of new material, including numerous specific results that have not yet appeared in the mathematical literature, as far as we are aware.

This work is divided into two volumes, each of which can stand by itself. This volume, *Mathematics by Experiment: Plausible Reasoning in the 21st Century*, presents the rationale and historical context of experimental

mathematics, and then presents a series of examples that exemplify the experimental methodology. We include in this volume a reprint of an article co-authored by one of us that complements this material. The second book, *Experimentation in Mathematics: Computational Paths to Discovery*, continues with several chapters of additional examples. Both volumes include a chapter on numerical techniques relevant to experimental mathematics.

Each volume is targeted to a fairly broad cross-section of mathematically trained readers. Most of this volume should be readable by anyone with solid undergraduate coursework in mathematics. Most of the second volume should be readable by persons with upper-division undergraduate or graduate-level coursework. None of this material involves highly abstract or esoteric mathematics.

The subtitle of this volume is taken from George Polya's well-known work, *Mathematics and Plausible Reasoning* [235]. This two-volume work has been enormously influential—if not uncontroversial—not only in the field of artificial intelligence, but also in the mathematical education and pedagogy community.

Some programming experience is valuable to address the material in this book. Readers with no computer programming experience are invited to try a few of our examples using commercial software such as *Mathematica* and *Maple*. Happily, much of the benefit of computational-experimental mathematics can be obtained on any modern laptop or desktop computer—a major investment in computing equipment and software is not required.

Each chapter concludes with a section of commentary and exercises. This permits us to include material that relates to the general topic of the chapter, but which does not fit nicely within the chapter exposition. This material is not necessarily sorted by topic nor graded by difficulty, although some hints, discussion and answers are given. This is because mathematics in the raw does not announce, “I am solved using such and such a technique.” In most cases, half the battle is to determine how to start and which tools to apply.

We should mention two recent books on mathematical experimentation: [158] and [203]. In both cases, however, the focus and scope centers on the teaching of students and thus is quite different from ours.

We are grateful to our colleagues Victor Adamchik, Heinz Bauschke, Peter Borwein, David Bradley, Gregory Chaitin, David and Gregory Chudnovsky, Robert Corless, Richard Crandall, Richard Fateman, Greg Fee, Helaman Ferguson, Steven Finch, Ronald Graham, Andrew Granville, Christoph Haenel, David Jeffrey, Jeff Joyce, Adrian Lewis, Petr Lisonek, Russell Luke, Mathew Morin, David Mumford, Andrew Odlyzko, Hristo Sendov, Luis Serrano, Neil Sloane, Daniel Rudolph, Asia Weiss, and John Zucker who were kind enough to help us prepare and review material for

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Experimental Mathematics Web Site

The authors have established a web site containing an updated collection of links to many of the URLs mentioned in the two volumes, plus errata, software, tools, and other web useful information on experimental mathematics. This can be found at the following URL:

<http://www.experimentalmath.info>

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David H. Bailey

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Expanded Second Edition

In this edition, in addition to correcting various minor infelicities and updating references, we have replaced the original Chapter 7 (which was a reprint of a philosophical article [76]) by roughly 100 pages of new material. We wish to thank Peter Borwein, David Bradley, David Broadhurst, Marc Chamberland, O-Yeat Chan, John Cosgrave, Richard Crandall, Karl Dilcher, Frank Garvan, John Holte, Manuel Kauers, Dante Manna, Veronica Pillwein, Mark Pinsky, Andrew Shouldice, Fernando Villegas, and Stan Wagon, among those who have provided interesting material for this new chapter. As before, our thanks go to our friends and editors at A K Peters for their support and care of our work.

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1

What is Experimental Mathematics?

The computer has in turn changed the very nature of mathematical experience, suggesting for the first time that mathematics, like physics, may yet become an empirical discipline, a place where things are discovered because they are seen.

– David Berlinski, “Ground Zero: A Review of The Pleasures of Counting, by T. W. Koerner,” 1997

If mathematics describes an objective world just like physics, there is no reason why inductive methods should not be applied in mathematics just the same as in physics.

– Kurt Gödel, *Some Basic Theorems on the Foundations*, 1951

1.1 Background

One of the greatest ironies of the information technology revolution is that while the computer was conceived and born in the field of pure mathematics, through the genius of giants such as John von Neumann and Alan Turing, until recently this marvelous technology had only a minor impact within the field that gave it birth.

This has not been the case in applied mathematics, as well as in most other scientific and engineering disciplines, which have aggressively integrated computer technology into their methodology. For instance, physicists routinely utilize numerical simulations to study exotic phenomena ranging from supernova explosions to big bang cosmology—phenomena that in many cases are beyond the reach of conventional laboratory experimentation. Chemists, molecular biologists, and material scientists make use of sophisticated quantum-mechanical computations to unveil the world of atomic-scale phenomena. Aeronautical engineers employ large-scale fluid dynamics calculations to design wings and engines for jet aircraft. Geologists and environmental scientists utilize sophisticated signal processing computations to probe the earth’s natural resources. Biologists har-

ness large computer systems to manage and analyze the exploding volume of genome data. And social scientists—economists, psychologists, and sociologists—make regular use of computers to spot trends and inferences in empirical data.

In the late 1980s, recognizing that its members were lagging behind in embracing computer technology, the American Mathematical Society began a regular “Computers and Mathematics” section in the monthly newsletter, *Notices of the American Mathematical Society*, edited at first by Jon Barwise and subsequently by Keith Devlin. This continued until the mid-1990s and helped to convince the mathematical community that the computer can be a useful research tool. In 1992, a new journal, *Experimental Mathematics*, was launched, founded on the belief “that theory and experiment feed on each other, and that the mathematical community stands to benefit from a more complete exposure to the experimental process.” It encouraged the submission of algorithms, results of experiments, and descriptions of computer programs, in addition to formal proofs of new results [135].

Perhaps the most important advancement along this line is the development of broad spectrum mathematical software products such as *Mathematica* and *Maple*. These days, many mathematicians are highly skilled with these tools and use them as part of their day-to-day research work. As a result, we are starting to see a wave of new mathematical results discovered partly or entirely with the aid of computer-based tools. Further developments in hardware (the gift of Moore’s Law of semiconductor technology), software tools, and the increasing availability of valuable Internet-based facilities, are all ensuring that mathematicians will have their day in the computational sun.

This new approach to mathematics—the utilization of advanced computing technology in mathematical research—is often called *experimental mathematics*. The computer provides the mathematician with a “laboratory” in which he or she can perform experiments: analyzing examples, testing out new ideas, or searching for patterns. Our book is about this new, and in some cases not so new, way of doing mathematics. To be precise, by experimental mathematics, we mean the methodology of doing mathematics that includes the use of computations for:

1. Gaining insight and intuition.
2. Discovering new patterns and relationships.
3. Using graphical displays to suggest underlying mathematical principles.
4. Testing and especially falsifying conjectures.

5. Exploring a possible result to see if it is worth formal proof.
6. Suggesting approaches for formal proof.
7. Replacing lengthy hand derivations with computer-based derivations.
8. Confirming analytically derived results.

Note that the above activities are, for the most part, quite similar to the role of laboratory experimentation in the physical and biological sciences. In particular, they are very much in the spirit of what is often termed “computational experimentation” in physical science and engineering, which is why we feel the qualifier “experimental” is particularly appropriate in the term experimental mathematics.

We should note that one of the more valuable benefits of the computer-based experimental approach in modern mathematics is its value in rejecting false conjectures (Item 4): A single computational example can save countless hours of human effort that would otherwise be spent attempting to prove false notions.

With regards to Item 5, we observe that mathematicians generally do not know during the course of research how it will pan out, but nonetheless must, in a conventional mathematical approach, prove all the pieces along the way as assurance that the project makes sense and remains on course. The methods of experimental mathematics allow mathematicians to maintain a reasonable level of assurance without nailing down all the lemmas the first time through. At the end of the day, they can decide if the result merits proof. If it is not the answer that was sought, or if it is simply not interesting enough, much less time will have been spent coming to this conclusion.

Many mathematicians remain uncomfortable with the appearance in published articles of expressions such as “proof by *Mathematica*” or “established by *Maple*” (see Item 7 above). There is, however, a clear trend in this direction, and it seems to us to be both futile and counterproductive to resist it. In Chapter 7 we will further explore the nature of mathematical experimentation and proof.

1.2 Complexity Considerations

Gordon Moore, the co-founder of Intel Corporation, noted in a 1965 article

The complexity for minimum component costs has increased at a rate of roughly a factor of two per year. . . . Certainly over the short

term this rate can be expected to continue, if not to increase. Over the longer term, the rate of increase is a bit more uncertain, although there is no reason to believe it will not remain nearly constant for at least 10 years. [219]

With these sentences, Moore stated what is now known as Moore's Law, namely the observation that semiconductor technology approximately doubles in capacity and overall performance roughly every 18 to 24 months (not quite every year as Moore predicted above). This trend has continued unabated for nearly 40 years, and, according to Moore and other industry analysts, there is still no end in sight—at least another ten years is assured [2]. This astounding record of sustained exponential progress has no peer in the history of technology. What's more, we will soon see mathematical computing tools implemented on parallel computer platforms, which will provide even greater power to the research mathematician.

However, we do not suggest that amassing huge amounts of processing power can solve all mathematical problems, even those that are amenable to computational analysis. There are doubtless some cases where a dramatic increase in computation could, by itself, result in significant breakthroughs, but it is easier to find examples where this is unlikely to happen.

For example, consider Clement Lam's 1991 proof of the nonexistence of a finite projective plane of order ten [200]. This involved a search for a configuration of $n^2 + n + 1$ points and equally many lines. Lam's computer program required thousands of hours of run time on a Cray computer system. Lam estimates that the next case ($n = 18$) susceptible to his methods would take millions of years on any conceivable architecture.

Along this line, although a certain class of computer-based mathematical analysis is amenable to “embarrassingly parallel” (the preferred term is now “naturally parallel”) processing, these tend not to be problems of central interest in mathematics. A good example of this is the search for Mersenne primes, namely primes of the form $2^n - 1$ for integer n . While such computations are interesting demonstrations of mathematical computation, they are not likely to result in fundamental breakthroughs. By contrast let us turn to perhaps the most fundamental of current algorithmic questions.

The P versus NP problem. (This discussion is taken from [67].) Of the seven million-dollar Millennium Prize problems, the one that is most germane to our present voyage is the so-called “P versus NP problem,” also known as the “ $P \neq NP$ ” problem. We quote from the discussion on the Clay web site:

It is Saturday evening and you arrive at a big party. Feeling shy, you wonder whether you already know anyone in the room. Your host

proposes that you must certainly know Rose, the lady in the corner next to the dessert tray. In a fraction of a second you are able to cast a glance and verify that your host is correct. However, in the absence of such a suggestion, you are obliged to make a tour of the whole room, checking out each person one by one, to see if there is anyone you recognize. This is an example of the general phenomenon that generating a solution to a problem often takes far longer than verifying that a given solution is correct. Similarly, if someone tells you that the number 13, 717, 421 can be written as the product of two smaller numbers, you might not know whether to believe him, but if he tells you that it can be factored as 3607 times 3803, then you can easily check that it is true using a hand calculator. One of the outstanding problems in logic and computer science is determining whether questions exist whose answer can be quickly checked (for example by computer), but which require a much longer time to solve from scratch (without knowing the answer). There certainly seem to be many such questions. But so far no one has proved that any of them really does require a long time to solve; it may be that we simply have not yet discovered how to solve them quickly. Stephen Cook formulated the P versus NP problem in 1971.

Although in many instances one may question the practical distinction between polynomial and nonpolynomial algorithms, this problem really is central to our current understanding of computing. Roughly it conjectures that many of the problems we currently find computationally difficult must *per force* be that way. It is a question about methods, not about actual computations, but it underlies many of the challenging problems one can imagine posing. A question that requests one to “compute such and such a sized incidence of this or that phenomena” always risks having the answer, “It’s just not possible,” because $P \neq NP$.

With the “NP” caveat (though factoring is difficult it is not generally assumed to be in the class of NP-hard problems), let us offer two challenges that are far fetched, but not inconceivable, goals for the next few decades.

First Challenge. Design an algorithm that can reliably factor a random thousand digit integer.

Even with a huge effort, current algorithms get stuck at about 150 digits. Details can be found at <http://www.rsasecurity.com/rsalabs/node.asp?id=2094> where the current factoring challenges are listed. One possible solution to the factorization problem may come through quantum computing, using an algorithm found by Peter Shor in 1994 [258]. However, it is still not clear whether quantum phenomenon can be harnessed on the scale required for this algorithm to be practical.

With regards to cash prizes, there is also \$100,000 offered for any honest 10,000,000 digit prime: <http://www.mersenne.org/prime.htm>.

Primality checking is currently easier than factoring, and there are some very fast and powerful *probabilistic* primality tests—much faster than those providing “certificates” of primality. There is also the recently discovered “AKS” deterministic polynomial time algorithm for primality, whose implementations, as we note in Section 7.2 of the second volume, keep improving.

Given that any computation has potential errors due to: (i) subtle (or even not-so-subtle) programming bugs, (ii) compiler errors, (iii) system software errors, and (iv) undetected hardware integrity errors, it seems increasingly pointless to distinguish between these two types of primality tests. Many would take their chances with a $(1 - 10^{-100})$ probability statistic over a “proof” any day (more on this topic is presented in Section 7.2 of the second volume).

The above questions are intimately related to the Riemann Hypothesis and its extensions, though not obviously so. They are also critical to issues of Internet security. If someone learns how to rapidly factor large numbers, then many current security systems are no longer secure.

Many old problems lend themselves to extensive exploration. One example that arose in signal processing is called the *Merit Factor problem*, and is due in large part to Marcel Golay with closely related versions due to Littlewood and to Erdős. It has a long pedigree though certainly not as elevated as the Riemann Hypothesis.

The problem can be formulated as follows. Suppose \mathcal{A}_n consists of all sequences $(a_0 = 1, a_1, \dots, a_n)$ of length $n + 1$ where each a_i is restricted to 1 or -1 , for $i > 0$. If $c_k = \sum_{j=0}^{n-k} a_j a_{j+k}$, then the problem is to minimize $\sum_{k=-n}^n c_k^2$ over \mathcal{A}_n for each fixed n . This is discussed at length in [82].

Minima have been found up to about $n = 50$. The search space of sequences of size 50 is $2^{50} \approx 10^{15}$, which approaches the limit of the very large-scale calculations feasible today. The records use a branch and bound algorithm which grows more or less like 1.8^n . This is marginally better than the naive 2^n growth of a completely exhaustive search but is still painfully exponential.

Second Challenge. Find the minima in the merit factor problem for sizes $n \leq 100$.

The best hope for a solution lies in development of better algorithms. The problem is widely acknowledged as a very hard problem in combinatorial optimization, but it isn’t known to be in one of the recognized hard classes like *NP*. The next best hope is a radically improved computer technology, perhaps quantum computing. And there is always a remote chance that analysis will lead to a mathematical solution.

1.3 Proof versus Truth

In any discussion of an experimental approach to mathematical research, the questions of reliability and standards of proof justifiably come to center stage. We certainly do not claim that computations utilized in an experimental approach to mathematics by themselves constitute rigorous proof of the claimed results. Rather, we see the computer primarily as an exploratory tool to discover mathematical truths, and to suggest avenues for formal proof.

For starters, it must be acknowledged that no amount of straightforward case checking constitutes a proof. For example, the “proof” of the Four Color Theorem in the 1970s, namely that every planar map can be colored with four colors so adjoining countries are never the same color, was considered a proof because prior mathematical analysis had reduced the problem to showing that a large but finite number of bad configurations could be ruled out. The “proof” was viewed as somewhat flawed because the case analysis was inelegant, complicated and originally incomplete (this computation was recently redone after a more satisfactory analysis). Though many mathematicians still yearn for a simple proof, there is no particular reason to believe that all elegant true conjectures have elegant proofs. What’s more, given Gödel’s result, some may have no proofs at all.

Nonetheless, we feel that in many cases computations constitute very strong evidence, evidence that is at least as compelling as some of the more complex formal proofs in the literature. Prominent examples include: (1) the determination that the Fermat number $F_{24} = 2^{2^{24}} + 1$ is composite, by Crandall, Mayer, and Papadopoulos [118, page 219]; (2) the recent computation of π to more than one trillion decimal digits by Yasumasa Kanada and his team; and (3) the Internet-based computation of binary digits of π beginning at position one quadrillion organized by Colin Percival. These are among the largest computations ever done, mathematical or otherwise (the π computations will be described in greater detail in Chapter 3). Given the numerous possible sources of error, including programming bugs, hardware bugs, software bugs, and even momentary cosmic-ray induced glitches (all of which are magnified by the sheer scale of these computations), one can very reasonably question the validity of these results.

But for exactly such reasons, computations such as these typically employ very strong validity checks. For example, the Crandall-Mayer-Papadopoulos computation employed a “wavefront” scheme. Here a faster computer system computed a chain of squares modulo F_{24} , such as $3^{2^{1000000}} \bmod F_{24}$, $3^{2^{2000000}} \bmod F_{24}$, $3^{2^{3000000}} \bmod F_{24}$, \dots . Then each of a set of slower computers started with one of these intermediate values, squared it

1,000,000 times modulo F_{24} , and checked to see if the result (a 16-million-bit integer) precisely reproduced the next value in the chain. If it did, then this is very strong evidence that both computations were correct. If not, then the process was repeated [118, page 219].

In the case of computations of digits of π , it has been customary for many years to verify a result either by repeating the computation using a different algorithm, or by repeating with a slightly different index position. For example, if one computes hexadecimal digits of π beginning at position one trillion (we shall see how this can be done in Chapter 3), then this can be checked by repeating the computation at hexadecimal position one trillion minus one. It is easy to verify (see Algorithm 3.4 in Section 3.4) that these two calculations take almost completely different trajectories, and thus can be considered “independent.” If both computations generate 25 hexadecimal digits beginning at the respective positions, then 24 digits should perfectly overlap. If these 24 hexadecimal digits do agree, then we can argue that the probability that these digits are in error, in a very strong (albeit heuristic) sense, is roughly one part in $16^{24} \approx 7.9 \times 10^{28}$, a figure much larger even than Avogadro’s number (6.022×10^{23}). Percival’s actual computation of the quadrillionth binary digit (i.e., the 250 trillionth hexadecimal digit) of π was verified by a similar scheme, which for brevity we have simplified here.

Kanada and his team at the University of Tokyo, who just completed a computation of the first 1.24 trillion decimal digits of π , employed an even more impressive validity check (Kanada’s calculation will be discussed in greater detail in Section 3.1). They first computed more than one trillion hexadecimal digits, using two different formulas. The hexadecimal digit string produced by both of these formulas, beginning at hex digit position 1,000,000,000,001, was **B4466E8D21 5388C4E014**. Next, they employed the algorithm, mentioned in the previous paragraph and described in more detail in Chapter 3, which permits one to directly compute hexadecimal digits beginning at a given position (in this case 1,000,000,000,001). This result was **B4466E8D21 5388C4E014**. Needless to say, these two sets of results, obtained by utterly different computational approaches, are in complete agreement. After this step, they converted the hexadecimal expansion to decimal, then back to hexadecimal as a check. When this final check succeeded, they felt safe to announce their results.

As a rather different example, a computation jointly performed by one of the present authors and David Broadhurst, a British physicist, discovered a previously unknown integer relation involving a set of 125 real constants associated with the largest real root of Lehmer’s polynomial [34]. This computation was performed using 50,000 decimal digit arithmetic and required 44 hours on 32 processors of a Cray T3E parallel supercomputer.

The 125 integer coefficients discovered by the program ranged in size up to 10^{292} . The certification of this relation to 50,000 digit precision was thus at least 13,500 decimal digits beyond the level ($292 \times 125 = 36,500$) that could reasonably be ascribed to numerical roundoff error. This result was separately affirmed by a computation on a different computer system, using 59,000-digit arithmetic, or roughly 22,500 decimal digits beyond the level of plausible roundoff error.

Independent checks and extremely high numerical confidence levels still do not constitute formal proofs of correctness. What's more, we shall see in Section 1.4 of the second volume some examples of "high-precision frauds," namely "identities" that hold to high precision, yet are not precisely true. Even so, one can argue that many computational results are as reliable, if not more so, than a highly complicated piece of human mathematics. For example, perhaps only 50 or 100 people alive can, given enough time, digest *all* of Andrew Wiles' extraordinarily sophisticated proof of Fermat's Last Theorem. If there is even a one percent chance that each has overlooked the same subtle error (and they may be psychologically predisposed to do so, given the numerous earlier results that Wiles' result relies on), then we must conclude that computational results are in many cases actually *more* secure than the proof of Fermat's Last Theorem.

Richard Dedekind's marvelous book, *Two Essays on Number Theory* [129], originally published in 1887, provides a striking example of how the nature of what is a satisfactory proof changes over time. In this work, Dedekind introduces Dedekind cuts and a modern presentation of the construction of the reals (see Item 2 at the end of this chapter). In the second essay, "The Nature and Meaning of Numbers," an equally striking discussion of finite and infinite sets takes place. Therein, one is presented with Theorem 66:

Theorem. There exist infinite systems.

Proof. My own realm of thoughts, i.e., the totality S of all things, which can be objects of my thought, is infinite. For if s signifies an element of S , then is the thought s' , that s can be object of my thought, itself an element of S . If we regard this as transform $\phi(s)$ of the element s then has the transformation ϕ of S , thus determined, the property that the transform S' is part of S ; and S' is certainly proper part of S , because there are elements in S (e.g., my own ego) which are different from such thought s' and therefore are not contained in S' . Finally, it is clear that if a, b are different elements of S , their transformation ϕ is a distinct (similar) transformation (26). Hence S is infinite, which was to be proved.

A similar presentation is found in §13 of the *Paradoxes des Unendlichen*, by Bolzano (Leipzig, 1851). Needless to say, such a "proof" would not be

acceptable today. In our modern formulation of mathematics there is an *Axiom of Infinity*, but recall that this essay predates the publications of Frege and Russell and the various paradoxes of modern set theory.

Some other examples of this sort are given by Judith Grabiner, who for instance compares Abel's comments on the lack of rigor in 18th-century arguments with the standards of Cauchy's 19th-century *Cours d'analyse* [151].

1.4 Paradigm Shifts

We acknowledge that the experimental approach to mathematics that we propose will be difficult for some in the field to swallow. Many may still insist that mathematics is all about formal proof, and from their viewpoint, computations have no place in mathematics. But in our view, mathematics is not ultimately about formal proof; it is instead about secure mathematical knowledge. We are hardly alone in this regard—many prominent mathematicians throughout history have either exemplified or explicitly espoused such a view.

Gauss expressed an experimental philosophy, and utilized an experimental approach on numerous occasions. In the next section, we shall present one significant example. Examples from de Morgan, Klein, and others will be given in subsequent sections.

Georg Friedrich Bernhard Riemann (1826–1866) was one of the most influential scientific thinkers of the past 200 years. However, he proved very few theorems, and many of the proofs that he did supply were flawed. But his conceptual contributions, such as Riemannian geometry and the Riemann zeta function, as well as his contributions to elliptic and Abelian function theory, were epochal.

Jacques Hadamard (1865–1963) was perhaps the greatest mathematician to think deeply and seriously about cognition in mathematics. He is quoted as saying “. . . in arithmetic, until the seventh grade, I was last or nearly last,” which should give encouragement to many young students. Hadamard was both the author of *The Psychology of Invention in the Mathematical Field* [160], a 1945 book that still rewards close inspection, and co-prover of the Prime Number Theorem in 1896, which stands as one of the premier results of 19th century mathematics and an excellent example of a result whose discovery and eventual proof involved detailed computation and experimentation. He nicely declared:

The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it. (J. Hadamard, from E. Borel, “Lecons sur la theorie des fonctions,” 1928, quoted in [234])

G. H. Hardy was another of the 20th century's towering figures in mathematics. In addition to his own mathematical achievements in number theory, he is well known as the mentor of Ramanujan. In his Rouse Ball lecture in 1928, Hardy emphasized the intuitive and constructive components of mathematical discovery:

I have myself always thought of a mathematician as in the first instance an observer, a man who gazes at a distant range of mountains and notes down his observations. . . . The analogy is a rough one, but I am sure that it is not altogether misleading. If we were to push it to its extreme we should be led to a rather paradoxical conclusion; that we can, in the last analysis, do nothing but point; that proofs are what Littlewood and I call gas, rhetorical flourishes designed to affect psychology, pictures on the board in the lecture, devices to stimulate the imagination of pupils. This is plainly not the whole truth, but there is a good deal in it. The image gives us a genuine approximation to the processes of mathematical pedagogy on the one hand and of mathematical discovery on the other; it is only the very unsophisticated outsider who imagines that mathematicians make discoveries by turning the handle of some miraculous machine. Finally the image gives us at any rate a crude picture of Hilbert's metamathematical proof, the sort of proof which is a ground for its conclusion and whose object is to convince. [87, Preface]

As one final example, in the modern age of computers, we quote John Milnor, a contemporary Fields medalist:

If I can give an abstract proof of something, I'm reasonably happy. But if I can get a concrete, computational proof and actually produce numbers I'm much happier. I'm rather an addict of doing things on computer, because that gives you an explicit criterion of what's going on. I have a visual way of thinking, and I'm happy if I can see a picture of what I'm working with. [241, page 78]

We should point out that paradigm shifts of this sort in scientific research have always been difficult to accept. For example, in the original 1859 edition of *Origin of the Species*, Charles Darwin wrote,

Although I am fully convinced of the truth of the views given in this volume . . . , I by no means expect to convince experienced naturalists whose minds are stocked with a multitude of facts all viewed, during a long course of years, from a point of view directly opposite to mine. . . . [B]ut I look with confidence to the future—to young and rising naturalists, who will be able to view both sides of the question with impartiality. [122, page 453]

In the 20th century, a very similar sentiment was expressed by Max Planck regarding quantum physics:

[A] new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents die and a new generation grows up that is familiar with it. [232, page 33–34]

Thomas Kuhn observed in his epochal work *The Structure of Scientific Revolutions*,

I would argue, rather, that in these matters neither proof nor error is at issue. The transfer of allegiance from paradigm to paradigm is a conversion experience that cannot be forced. [195, page 151]

Two final quotations deal with the dangers of overreliance on tradition and “authority” in scientific research. The first is an admonition by the early English scholar-scientist Robert Record, in his 1556 cosmology textbook *The Castle of Knowledge*:

No man can worthily praise Ptoleme . . . yet muste ye and all men take heed, that both in him and in all mennes workes, you be not abused by their autoritye, but evermore attend to their reasons, and examine them well, ever regarding more what is saide, and how it is proved, than who saieth it, for autorite often times deceaveth many menne. [138, page 47]

The following is taken from an intriguing, recently published account of why one of the most influential articles of modern mathematical economics, which in fact later led to a Nobel Prize for its authors (John R. Hicks and Kenneth J. Arrow), was almost not accepted for publication:

[T]o suggest that the normal processes of scholarship work well on the whole and in the long run is in no way contradictory to the view that the processes of selection and sifting which are essential to the scholarly process are filled with error and sometimes prejudice. (Kenneth Arrow [285])

1.5 Gauss, the Experimental Mathematician

Carl Friedrich Gauss once confessed

I have the result, but I do not yet know how to get it. [11, page 115]

Gauss was particularly good at seeing meaningful patterns in numerical data. When just 14 or 15 years old, he conjectured that $\pi(n)$, the number of primes less than n , is asymptotically approximated by $n/\log n$. This conjecture is, of course, the Prime Number Theorem, eventually proved by Hadamard and de la Vallée Poussin in 1896. This will be discussed in greater detail in Section 2.8.

Here is another example of Gauss's prowess at "mental experimental mathematics." 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: $a_0 = 1$, $b_0 = \sqrt{2}$;

$$a_{n+1} = \frac{a_n + b_n}{2}, \quad b_{n+1} = \sqrt{a_n b_n}. \quad (1.1)$$

The sequences (a_n) and (b_n) have the limit 1.1981402347355922074... in common. Based on this purely computational observation, Gauss was able to conjecture and subsequently prove that the integral is indeed equal to this common limit. It was a remarkable result, of which he wrote in his diary (see [74, pg. 5] and below) "[the result] will surely open up a whole new field of analysis." He was right. It led to the entire vista of 19th century elliptic and modular function theory.

We reproduce the relevant pages from his diary as Figures 1.1 and 1.2. The first shows the now familiar hypergeometric series which, along with the arithmetic-geometric mean iteration, we discuss in some detail in Section 5.6.2.

In Figure 1.2, an excited Gauss writes:

Novus in analysi campus se nobis aperuit, scilicet investigatio functionem etc. (October 1798) [A new field of analysis has appeared to us, evidently in the study of functions etc.]

And in May 1799 (a little further down the page), he writes:

Terminum medium arithmetico-geometricum inter 1 et (root 2) esse pi/omega usque ad figuram undecimam comprobavimus, qua re demonstrata prorsus novus campus in analysi certo aperietur. [We have shown the limit of the arithmetical-geometric mean between 1 and root 2 to be pi/omega up to eleven figures, which on having been demonstrated, a whole new field in analysis is certain to be opened up.]

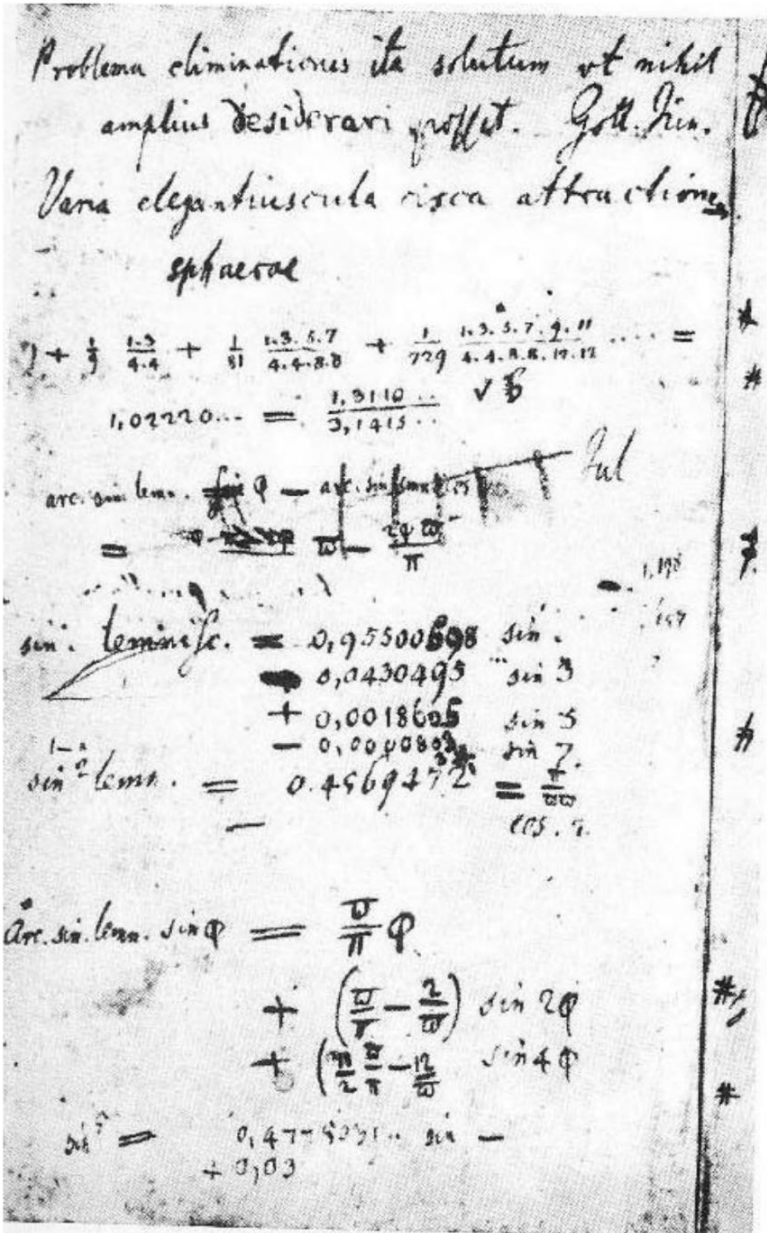


Figure 1.1. Gauss on the lemniscate.

Hic lenitate, et quam diffime omnes expectati-
 ones superantia acquisitionibus et quibus
 per methodos suae campum propus-
 sionum nobis aperiant. Gott. Jul.

Solutio problematis ballistici Gott. Jul.

Comitarum theoriam perfectiorem reddidi Gott. Jul.

Novus in analysi campus de nobis aperuit,
 scilicet investigatio functionum etc.

Formas superiores considerare coepimus
 Pr. Febr. 1777

Formulas novas exactas pro parallaxi
 eruius ——— Pr. Apr. 8.

Terminum medium arithmetico-geometricum
 inter 1 et $\sqrt{2}$ esse = $\frac{\pi}{10}$ usque
 ad figuram undecimam comprobavimus, quare
 demonstrata proinde novus campus in analysi
 certo aperietur Pr. Maio.

In principiis Geometriae egregios progressus
 fecimus Pr. Sept.

Circa terminos medios arithmetico-geometricos
 multae novae determinationes. Pr. Novemb.

Figure 1.2. Gauss on the arithmetic-geometric mean.

1.6 Geometric Experiments

Augustus de Morgan (1806–71), the first President of the London Mathematical Society, was equally influential as an educator and a researcher [242]. As the following two quotes from De Morgan show, neither a pride in numerical skill nor a desire for better geometric tools is new. De Morgan like many others saw profound differences between two and three dimensions:

Considerable obstacles generally present themselves to the beginner, in studying the elements of Solid Geometry, from the practice which has hitherto uniformly prevailed in this country, of never submitting to the eye of the student, the figures on whose properties he is reasoning, but of drawing perspective representations of them upon a plane. . . . I hope that I shall never be obliged to have recourse to a perspective drawing of any figure whose parts are not in the same plane.

There is considerable evidence that young children see more naturally in three than two dimensions.

Elsewhere, de Morgan celebrates:

In 1831, Fourier's posthumous work on equations showed 33 figures of solution, got with enormous labor. Thinking this is a good opportunity to illustrate the superiority of the method of W. G. Horner, not yet known in France, and not much known in England, I proposed to one of my classes, in 1841, to beat Fourier on this point, as a Christmas exercise. I received several answers, agreeing with each other, to 50 places of decimals. In 1848, I repeated the proposal, requesting that 50 places might be exceeded: I obtained answers of 75, 65, 63, 58, 57, and 52 places.

Angela Vierling's web page <http://math.bu.edu/people/angelav/projects/models> describes well the 19th century desire for aids to visualization:

During many of these investigations, models were built to illustrate properties of these surfaces. The construction and study of plaster models was especially popular in Germany (particularly in Göttingen under the influence of Felix Klein). Many of the models were mass produced by publishing houses and sold to mathematicians and mathematics departments all over the world. Models were built of many other types of surfaces as well, including surfaces arising from the study of differential geometry and calculus. Such models enjoyed a wonderful reception for a while, but after the 1920's production and interest waned.

Felix Klein, like De Morgan, was equally influential as researcher and as educator. These striking and very expensive models still exist in many university departments and can be viewed as a precursor to modern electronic visualization tools such as Rob Scharein's KnotPlot site <http://www.colab.sfu.ca/KnotPlot>, which now has a three dimensional "immersive reality" version, and the remarkable Electronic Geometry Models site <http://www.eg-models.de>.

While we will not do a great deal of geometry in this book, this arena has great potential for visualization and experimentation. Three beautiful theorems come to mind where visualization, in particular, plays a key role:

1. *Pick's theorem* on the area of a simple lattice polygon, P :

$$A(P) = I(P) + \frac{1}{2}B(P) - 1, \quad (1.2)$$

where $I(P)$ is the number of lattice points inside P and $B(P)$ is the number of lattice points on the boundary of P including the vertices.

2. Minkowski's seminal result in the geometry of numbers that *a symmetric convex planar body must contain a nonzero lattice point in its interior if its area exceeds four.*
3. Sylvester's theorem: *Given a noncollinear finite set in the plane, one can always draw a line through exactly two points of the set.*

In the case of Pick's theorem it is easy to think of a useful experiment (one of the present authors has invited students to do this experiment). It is reasonable to first hunt for a formula for acute-angled triangles. One can then hope to piece together the more general result by triangulating the polygon (even if it is nonconvex), and then clearly for right-angled triangles. Now place the vertices at $(n, 0)$, $(0, m)$, and $(0, 0)$ and write a few lines of code that separately totals the number of times (j, k) lies on the boundary lines or inside the triangle as j ranges between 0 and n and k between 0 and m . A table of results for small m and n will expose the result. For example, if we consider all right-angled triangles of height h and width w with area 30, we obtain:

$$\begin{bmatrix} h & w & A & I & B \\ 10 & 6 & 30 & 22 & 18 \\ 12 & 5 & 30 & 22 & 18 \\ 15 & 4 & 30 & 21 & 20 \\ 20 & 3 & 30 & 19 & 24 \\ 30 & 2 & 30 & 14 & 34 \\ 60 & 1 & 30 & 0 & 62 \end{bmatrix}. \quad (1.3)$$

It is more of a challenge to think of a useful experiment to determine that “4” is the right constant in Minkowski’s theorem. Both of these results are very accessibly described in [227].

James Sylvester, mentioned in Item 3 above, was president of the London Mathematical Society in the late 19th century. He once wrote, “The early study of Euclid made me a hater of geometry” [208]. Discrete geometry (now much in fashion as “computational geometry” and another example of very useful pure mathematics) was clearly more appealing to Sylvester. For Sylvester’s theorem (posed but not solved by Sylvester), one can imagine various Java applets but scattering a fair number of points on a sheet of white paper and using a ruler seems more than ample to get a sense of the truth of the result.

Sylvester’s conjecture was largely forgotten for 50 years. It was first established—“badly” in the sense that the proof is much more complicated than it needed to be—by Gallai (1943) and also by Paul Erdős, who named “the Book” in which God keeps elegant and aesthetically perfect proofs. Kelly’s proof, which was declared by Erdős to be “in the Book,” was actually published by Donald Coxeter in the *American Mathematical Monthly* in 1948 (this is a good example of how easily the archival record is often obscured). A marvellous eponymous book is [4]. It is chock full of proofs that are or should be in the book and, for example, gives six proofs of the infinitude of primes.

Proof Sketch. Let S be the given set of points. Consider the collection \mathcal{C} of pairs (L, p) , where L is a line through (at least two distinct) points in S and where p is a point in S not on L . Then \mathcal{C} is nonempty and contains only finitely many such pairs. Among those, pick (L, p) such that the distance from p to L is *minimal*. We claim that L harbors exactly two points from S .

Assume not, then, L contains 3 or more points. In Figure 1.3, L is represented as the horizontal line. Let q be the projection of p onto L . In Figure 1.3, we drew 3 points of S on L . Label these points a, b, c . (Two must be on one side of q .) Consider b and draw the line L' through p and either a or c , whichever line is closer to b . In Figure 1.3, L' is the slanted line. Then (L', b) belongs to \mathcal{C} and the distance from b to L' is strictly smaller than the distance from p to L . But this contradicts the choice of (L, p) . \square

As with the visual proof of the irrationality of $\sqrt{2}$, which we will give in Section 2.9, we see forcibly the power of the right *minimal configuration*.

Dirac conjectured that every sufficiently large set of n noncollinear points contains at least $n/2$ proper (or elementary) lines through exactly two points.

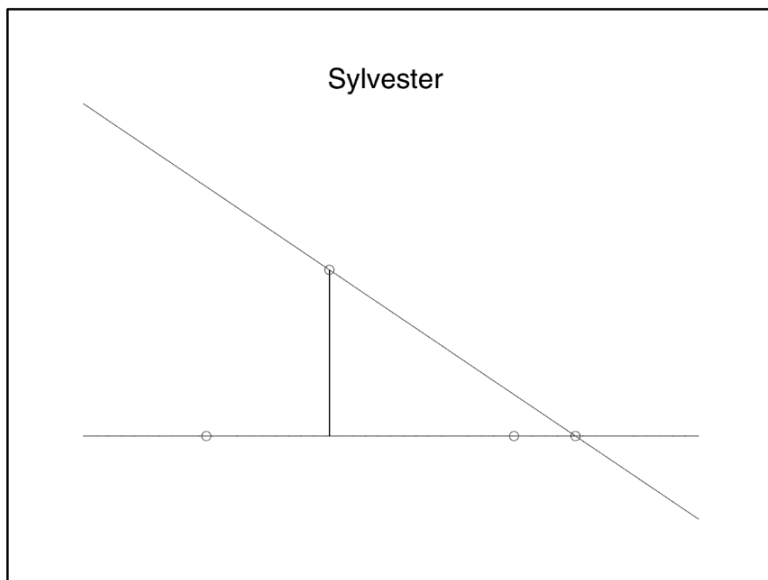


Figure 1.3. Kelly’s 1948 “Proof from the Book.”

By contrast,

The Desmic configuration, discovered by Stepanos in 1890, is [...] a configuration spanning 3-space, consisting of three tetrads of points, each two of the tetrads being in perspective from the four points of the third tetrad. This means that any line intersecting two of the tetrads also intersects the third. [81]

It is conjectured that in many senses this configuration (built from the corners of the cube and a point at infinity) is unique [81]. One can view the Desmic configuration as showing that the Sylvester-Gallai theorem “fails in three dimensions.”

Sylvester had a most colorful and somewhat difficult life which included a seminal role in the founding of Johns Hopkins University, and ended as the first Jewish Chair in Oxford. Educated in Cambridge, he could not graduate until 1871, when theological tests were finally abolished. This is engagingly described in *Oxford Figures* [138].

Along this line, readers may be interested in Figures 1.4 and 1.5, which are taken from Part VII of a 19th century experimental geometry book by the French educator Paul Bert. The intention was to make school geometry more intuitive and empirical, quite far from Euclid’s *Elements*.

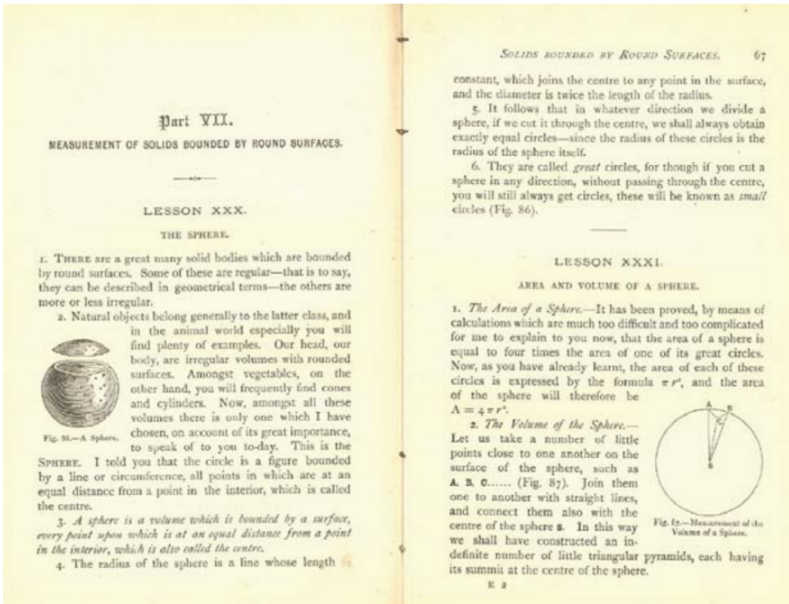


Figure 1.4. Paul Bert's 1886 experimental geometry text, pages 66–67.

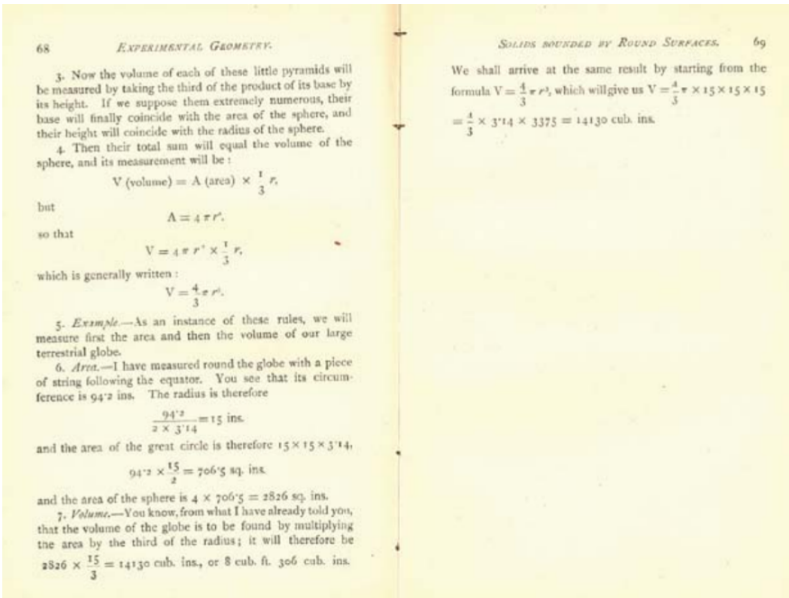


Figure 1.5. Paul Bert's text, pages 68–69.

A total of 94 teams, representing 25 different nations, submitted results. Twenty of these teams received a full 100 points (10 correct digits for each problem). Since these results were much better than expected, an initially anonymous donor, William J. Browning, provided funds for a \$100 award to each team. The present authors and Greg Fee entered, but failed to qualify for an award. The ten problems are:

1. What is $\lim_{\epsilon \rightarrow 0} \int_{\epsilon}^1 x^{-1} \cos(x^{-1} \log x) dx$?
2. A photon moving at speed 1 in the x - y plane starts at $t = 0$ at $(x, y) = (1/2, 1/10)$ heading due east. Around every integer lattice point (i, j) in the plane, a circular mirror of radius $1/3$ has been erected. How far from the origin is the photon at $t = 10$?
3. The infinite matrix A with entries $a_{11} = 1$, $a_{12} = 1/2$, $a_{21} = 1/3$, $a_{13} = 1/4$, $a_{22} = 1/5$, $a_{31} = 1/6$, etc., is a bounded operator on ℓ^2 . What is $\|A\|$?
4. What is the global minimum of the function $\exp(\sin(50x)) + \sin(60e^y) + \sin(70 \sin x) + \sin(\sin(80y)) - \sin(10(x+y)) + (x^2 + y^2)/4$?
5. Let $f(z) = 1/\Gamma(z)$, where $\Gamma(z)$ is the gamma function, and let $p(z)$ be the cubic polynomial that best approximates $f(z)$ on the unit disk in the supremum norm $\|\cdot\|_{\infty}$. What is $\|f - p\|_{\infty}$?
6. A flea starts at $(0, 0)$ on the infinite 2-D integer lattice and executes a biased random walk: At each step it hops north or south with probability $1/4$, east with probability $1/4 + \epsilon$, and west with probability $1/4 - \epsilon$. The probability that the flea returns to $(0, 0)$ sometime during its wanderings is $1/2$. What is ϵ ?
7. Let A be the 20000×20000 matrix whose entries are zero everywhere except for the primes $2, 3, 5, 7, \dots, 224737$ along the main diagonal and the number 1 in all the positions a_{ij} with $|i - j| = 1, 2, 4, 8, \dots, 16384$. What is the $(1, 1)$ entry of A^{-1} .
8. A square plate $[-1, 1] \times [-1, 1]$ is at temperature $u = 0$. At time $t = 0$ the temperature is increased to $u = 5$ along one of the four sides while being held at $u = 0$ along the other three sides, and heat then flows into the plate according to $u_t = \Delta u$. When does the temperature reach $u = 1$ at the center of the plate?
9. The integral $I(\alpha) = \int_0^2 [2 + \sin(10\alpha)] x^{\alpha} \sin(\alpha/(2-x)) dx$ depends on the parameter α . What is the value $\alpha \in [0, 5]$ at which $I(\alpha)$ achieves its maximum?

identify the sequence in Sloane. Confirm Euler's observation that for $n = 0, 1, \dots, 8$ that $3t_{n+1} - t_{n+2} = F_n(F_n + 1)$, where F_n is the n th Fibonacci number, but fails subsequently.

- (b) Consider the sequence u_n defined by $u_{n+2} := \lfloor \frac{1}{2} + u_{n+1}^2 / u_n \rfloor$ with $u_0 := 3, u_1 := 10$. Show that

$$\sum_{n \geq 0} u_n x^{n+1} = \frac{1}{1 - x(3 + x)}.$$

- (c) By contrast, consider $\{u_n\}$ defined by $u_{n+2} := \lfloor 1 + u_{n+1}^2 / u_n \rfloor$ with $u_0 := 8, u_1 := 55$. Consider also the rational function

$$\begin{aligned} R(x) &:= \frac{8 + 7x - 7x^2 - 7x^3}{1 - 6x - 7x^2 + 5x^3 + 6x^4} \\ &= 8 + 55x + 379x^2 + 2612x^3 + \dots \end{aligned}$$

and determine that the first time $[x^n]R(x)$ and u_n differ is for $n = 11056$. How far can you confirm the equality?

- (d) Consult Sloane's recursively defined sequences A006722 (6-Somos) and A003502 (Göbel). The first of the two sequences

$$a_n := (a_{n-1}a_{n-5} + a_{n-2}a_{n-4} + a_{n-3}^2) / a_{n-6}$$

for $n > 5$ with the first five values unity, provably takes only integer values, whereas the second one

$$a_{n+1} := \left(\sum_{k=0}^n a_k^2 \right) / n \text{ and } a_0 := 1$$

appears to only for n up to 43 (that is, the sequence is integral for $n < 44$ and the rest are not). As $a_{44} = 5.4093 \dots \times 10^{178485291567}$, it is impossible to deduce this via direct computation.

67. **Another matrix class.** Determine the probable closed form of the matrix sequence that begins

$$[1], \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix}, \begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & 9 \\ 3 & 9 & 19 \end{bmatrix}, \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 9 & 14 \\ 3 & 9 & 19 & 34 \\ 4 & 14 & 34 & 69 \end{bmatrix}, \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 5 & 9 & 14 & 20 \\ 3 & 9 & 19 & 34 & 55 \\ 4 & 14 & 34 & 69 & 125 \\ 5 & 20 & 55 & 125 & 251 \end{bmatrix}.$$