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Intuition 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.


The authors first met in 1985, when Bailey used the Borwein quartic algorithm for \( \pi \) 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 plunged 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* [47], 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 [88].

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* [167]. 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: [105] and [142]. In both cases, however, the focus and scope centers on the teaching of students and thus is quite different from ours.

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Preface

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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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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.


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 [87].

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

\[
\text{The complexity for minimum component costs has increased at a rate of roughly a factor of two per year. \ldots Certainly over the short}
\]
1. What is Experimental Mathematics?

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. [155]

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 [140]. 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 [44].) 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](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 [179]. 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](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 $A_n$ consists of all sequences $(a_0 = 1, a_1, \cdots, a_n)$ 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 $A_n$ for each fixed $n$. This is discussed at length in [55].

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 naïve $2^n$ 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 [79]; (2) the recent computation of \(\pi\) to more than one trillion decimal digits by Yasumasa Kanada and his team; and (3) the Internet-based computation of binary digits of \(\pi\) beginning at position one quadrillion organized by Colin Percival. These are among the largest computations ever done, mathematical or otherwise (the \(\pi\) 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 \(3^{2^{300000}} \mod F_{24}, 3^{2^{600000}} \mod F_{24}, 3^{2^{900000}} \mod F_{24}, \ldots\). 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 [79, page 187].

In the case of computations of digits of $\pi$, 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 $\pi$ 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 3.0 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 ($6.022 \times 10^{23}$). Percival’s actual computation of the quadrillionth binary digit (i.e., the 250 trillionth hexadecimal digit) of $\pi$ 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 $\pi$, 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 $B4466E8D215388C4E014$. 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 $B4466E8D215388C4E014$. 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 [22]. This computation was performed using 50,000 decimal digit arithmetic and required 44 hours on 32 processors of a Cray T3E parallel supercomputer.
1.3. Proof versus Truth

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* [84], 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 $\phi$ 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 $\phi$ 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* [99].

### 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* [106], 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 [166]*)
1.4. Paradigm Shifts

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. [58, 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. [170, 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. [80, 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. [164] 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. [134] 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 Ptolemy . . . 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. [90] 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 [191])

### 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. [8] 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:

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

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

The sequences $(a_n)$ and $(b_n)$ have the limit $1.1981402347355922074\ldots$ 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 [49, 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:

*Terminus medium arithmetico-geometricum inter 1 et (root 2) esse pi/omega usque ad figuram undcimam comprobavium, qua re demonstrata prorsus novus campus in analysi certo aperuit.* [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.]
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Figure 1.1. Gauss on the lemniscate.
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 [171]. 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](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.shu.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, \( P \):

\[
A(P) = I(P) + \frac{1}{2}B(P) - 1, \tag{1.2}
\]

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:

\[
\begin{bmatrix}
  h & w & A & I & B \\
  10 & 6 & 30 & 22 & 18 \\
  12 & 5 & 30 & 22 & 18 \\
  15 & 4 & 30 & 21 & 20 \\
  20 & 3 & 30 & 19 & 24 \\
  30 & 2 & 30 & 14 & 34 \\
  60 & 1 & 30 & 0 & 62 \\
\end{bmatrix} \tag{1.3}
\]
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 [161].

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” [146]. 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 [3]. 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 $C$ 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 $C$ 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 $C$ 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 $\sqrt{2}$, 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.
By contrast,

The Desmic configuration, discovered by Stephanos 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. \[54\]

It is conjectured that in many senses this configuration (built from the corners of the cube and a point at infinity) is unique \[54\]. 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 \[90\].

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

Figure 1.5. Paul Bert’s text, pages 68–69.
1.6. Geometric Experiments

1.6.1 On Picture-Writing

George Polya, in an engaging eponymous *American Mathematical Monthly* article, provides three compelling examples of converting pictorial representations of problems into generating function solutions [165]:

1. *In how many ways can you make change for a dollar?*

This leads to the (US currency) generating function

\[ \sum_{k=1}^{\infty} P_k x^k = \frac{1}{(1-x)(1-x^5)(1-x^{10})(1-x^{25})(1-x^{50})}, \]

which one can easily expand using a *Mathematica* command,

\[
\text{Series}\left[\frac{1}{(1-x)(1-x^5)(1-x^{10})(1-x^{25})(1-x^{50})}, \{x, 0, 100\}\right]
\]

to obtain \( P_{100} = 292 \) (242 for Canadian currency, which lacks a 50 cent piece). Polya’s illustration is shown in Figure 1.6.

2. *Dissect a polygon with \( n \) sides into \( n - 2 \) triangles by \( n - 3 \) diagonals and compute \( D_n \), the number of different dissections of this kind.*

This leads to the fact that the generating function for \( D_3 = 1, D_4 = 2, D_5 = 5, D_6 = 14, D_7 = 42, \ldots \)

\[ D(x) = \sum_{k=1}^{\infty} D_k x^k \]
1. What is Experimental Mathematics?

satisfies

\[ D(x) = x \left[ 1 + D(x) \right]^2, \]

whose solution is therefore

\[ D(x) = \frac{1 - 2x - \sqrt{1 - 4x}}{x}, \]

and \( D_{n+2} \) turns out to be the \( n \)-th Catalan number \( \frac{2^n}{n+1} \).

3. Compute \( T_n \), the number of different (rooted) trees with \( n \) knots.

The generating function of the \( T_n \) becomes a remarkable result due to Cayley:

\[
T(x) = \sum_{k=1}^{\infty} T_k x^k = x \prod_{k=1}^{\infty} (1 - x^k)^{-T_k},
\]

where remarkably the product and the sum share their coefficients. This produces a recursion for \( T_n \) in terms of \( T_1, T_2, \ldots, T_{n-1} \), which starts: \( T_1 = 1, T_2 = 1, T_3 = 2, T_4 = 4, T_5 = 9, T_6 = 20, \ldots \) We shall revisit such products in Section 4.2 of the second volume of this work.

In each case, Polya’s main message is that one can usefully draw pictures of the component elements—(a) in pennies, nickels dimes and quarters (plus loonies in Canada and half dollars in the US), (b) in triangles and (c) in the simplest trees (with the fewest knots).

1.7 Sample Problems of Experimental Math

In the January 2002 issue of SIAM News, Nick Trefethen of Oxford University presented ten diverse problems used in teaching graduate numerical analysis students at Oxford University, the answer to each being a certain real number. Readers were challenged to compute ten digits of each answer, with a $100 prize to the best entrant. Trefethen wrote, “If anyone gets 50 digits in total, I will be impressed.”

Success in solving these problems requires a broad knowledge of mathematics and numerical analysis, together with significant computational effort to obtain solutions and ensure correctness of the results. The strengths and limitations of Maple, Mathematica, MATLAB and other software tools are strikingly revealed in these exercises.
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 \( \lim_{\epsilon \to 0} \int_{\epsilon}^{1} x^{-1} \cos(x^{-1} \log x) \, dx \)?

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 \( \ell^2 \). 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 \( \epsilon \)?

7. Let \( A \) be the \( 20000 \times 20000 \) matrix whose entries are zero everywhere except for the primes \(2, 3, 5, 7, \cdots, 224737\) along the main diagonal and the number 1 in all the positions \( a_{ij} \) with \(|i - j| = 1, 2, 4, 8, \cdots, 16384\). 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 \( I(\alpha) = \int_0^\alpha [2 + \sin(10\alpha)]x^n \sin(\alpha/(2 - x)) \, dx \) depends on the parameter \( \alpha \). What is the value \( \alpha \in [0, 5] \) at which \( I(\alpha) \) achieves its maximum?
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10. A particle at the center of a $10 \times 1$ rectangle undergoes Brownian motion (i.e., 2-D random walk with infinitesimal step lengths) till it hits the boundary. What is the probability that it hits at one of the ends rather than at one of the sides?

These problems and their solutions are described in detail in a forthcoming book [40]. Answers correct to 40 digits are available at the URL http://web.comlab.ox.ac.uk/oucl/work/nick.trefethen/hundred.html

Inspired by this set of problems, the present authors have assembled a similar set of problems, similar in style to the SIAM/Oxford 100 Digit Challenge, but emphasizing the flavor of experimental mathematics. As in the above problem set, a real constant is defined in each case. The objective here is to produce at least 100 correct digits digits, so that a total of 1000 points can be earned. Several of these can be solved by fairly direct application of numerical computation, but others require mathematical analysis and reduction before computation can be done in reasonable time. Each problem provides an “extra credit” question, for which an additional 100 points may be earned. The maximum total score is thus 2000 points.

In each case, these problems can be solved with techniques presented either in this volume or in the companion volume. Answers, with references, can be found at the URL http://www.experimentalmath.info

1. Compute the value of $r$ for which the chaotic iteration $x_{n+1} = rx_n(1-x_n)$, starting with some $x_0 \in (0,1)$, exhibits a bifurcation between 4-way periodicity and 8-way periodicity.

Extra credit: This constant is an algebraic number of degree not exceeding 20. Find the minimal polynomial with integer coefficients that it satisfies.

2. Evaluate

$$
\sum_{(m,n,p) \neq 0} \frac{(-1)^{m+n+p}}{\sqrt{m^2 + n^2 + p^2}},
$$

where convergence means the limit of sums over the integer lattice points enclosed in increasingly large cubes surrounding the origin.

Extra credit: Identify this constant.

3. Evaluate the sum

$$
\sum_{k=1}^{\infty} \left( 1 - \frac{1}{2} + \cdots + (-1)^{k+1} \frac{1}{k} \right)^2 (k+1)^{-3}.
$$
1.7. Sample Problems of Experimental Math

Extra credit: Evaluate this constant as a multiterm expression involving well-known mathematical constants. This expression has seven terms, and involves $\pi$, $\log 2$, $\zeta(3)$, and $\text{Li}_5(1/2)$, where $\text{Li}_n(x) = \sum_{k>0} x^k/n^k$ is the polylogarithm of order $n$. For $n = 2, 3$ these are also called the dilogarithm and trilogarithm respectively.

*Hint:* The expression is “homogenous,” in the sense that each term has the same total “degree.” The degrees of $\pi$ and $\log 2$ are each 1, the degree of $\zeta(3)$ is 3, the degree of $\text{Li}_5(1/2)$ is 5, and the degree of $\alpha^n$ is $n$ times the degree of $\alpha$.

4. Evaluate

$$\prod_{k=1}^{\infty} \left[ 1 + \frac{\log k}{k(k+2)} \right]^{\frac{1}{\log_2 k}} = \prod_{k=1}^{\infty} k^{\left[ \frac{\log_2 \left( 1 + \frac{1}{k+1} \right) }{\log_2 k} \right]}.$$

Extra credit: Evaluate this constant in terms of a less-well-known mathematical constant.

5. Given $a, b, \eta > 0$, define

$$R_\eta(a, b) = \frac{a}{\eta + \frac{b^2}{\eta + \frac{4\omega^2}{\eta + \frac{9\omega^2}{\eta + \ldots}}}}.$$

Calculate $R_1(2, 2)$.

Extra credit: Evaluate this constant as a two-term expression involving a well-known mathematical constant.

6. Calculate the expected distance between two random points on different sides of the unit square.

*Hint:* This can be expressed in terms of integrals as

$$\frac{2}{3} \int_0^1 \int_0^1 \sqrt{x^2+y^2} \, dx \, dy + \frac{1}{3} \int_0^1 \int_0^1 \sqrt{1+(y-u)^2} \, du \, dy.$$

Extra credit: Express this constant as a three-term expression involving algebraic constants and an evaluation of the natural logarithm with an algebraic argument.
7. Calculate the expected distance between two random points on different faces of the unit cube. \textit{Hint:} This can be expressed in terms of integrals as
\[
\frac{4}{5} \int_0^1 \int_0^1 \int_0^1 \int_0^1 \sqrt{x^2 + y^2 + (z - w)^2} \, dw \, dy \, dz \\
+ \frac{1}{5} \int_0^1 \int_0^1 \int_0^1 \int_0^1 \sqrt{1 + (y - w)^2 + (z - w)^2} \, du \, dw \, dy \, dz.
\]
Extra credit: Express this constant as a six-term expression involving algebraic constants and two evaluations of the natural logarithm with algebraic arguments.

8. Calculate
\[
\int_0^\infty \cos(2x) \prod_{n=1}^\infty \cos \left( \frac{x}{n} \right) \, dx.
\]
Extra credit: Express this constant as an analytic expression. \textit{Hint:} It is not what it first appears to be.

9. Calculate
\[
\sum_{i>j>k>l>0} \frac{1}{i^3 j^3 k^3 l^3}.
\]
Extra credit: Express this constant as a single-term expression involving a well-known mathematical constant.

10. Evaluate
\[
W_1 = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{1}{3 - \cos(x) - \cos(y) - \cos(z)} \, dx \, dy \, dz.
\]
Extra credit: Express this constant in terms of the Gamma function.

1.8 Internet-Based Mathematical Resources

We list here some Internet-based resources that we have found useful in our research. We have selected those that we believe will be fairly permanent, but some may become defunct with the passage of time. An updated list of these URLs, with links, can be found at \url{http://www.experimentalmath.info}.
1.8. Internet-Based Mathematical Resources

**Institutional Sites**

1. American Institute of Mathematics:
   http://www.aimath.org

2. Canadian Mathematical Society’s KaBoL site:
   http://camel.math.ca/Kabol

3. Clay Mathematics Institute:
   http://www.claymath.org

4. Experimental Mathematics Journal:
   http://www.expmath.org

5. European Mathematical Society:
   http://elib.uni-osnabrueck.de

6. Mathematical Association of America Online:
   http://www.maa.org

7. Math-Net (International Mathematical Union):
   http://www.Math-Net.org

8. MathSciNet:
   http://e-math.ams.org/mathscinet

9. Society for Industrial and Applied Mathematics:
   http://www.siam.org

**Commercial Sites**

1. Apple Computer’s Advanced Computation Group research site:

2. The Cinderella interactive geometry site:
   http://www.cinderella.de

3. Integrals.com (operated by Wolfram Research):
   http://www.integrals.com

4. Maplesoft (*Maple*):
   http://www.maplesoft.com
   http://www.mapleapps.com

5. MathResources interactive dictionaries:
   http://www.mathresources.com
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6. Mathworks (MATLAB):
   http://www.mathworks.com

7. NEC’s CiteSeer database:
   http://citeseer.ist.psu.edu

8. Eric Weisstein’s World of Mathematics site:
   http://mathworld.wolfram.com

9. Wolfram Research, Inc. (Mathematica):
   http://www.wolfram.com

Noncommercial Software and Tools

1. Alf-Christian Achilles’ computer science bibliography:
   http://liinwww.ira.uka.de/bibliography

2. The Algorithm Project software library:
   http://algo.inria.fr/libraries/software.html

3. The ArXiv mathematics article database:
   http://front.math.ucdavis.edu

4. The Boyer-Moore theorem prover:
   http://www.cs.utexas.edu/users/moore/best-ideas/nqthm

5. The CECM Euler-zeta computation tool:
   http://www.cecm.sfu.ca/projects/ezface+

6. The CECM integer relation tool (see also Item 7):
   http://www.cecm.sfu.ca/projects/IntegerRelations

7. The CECM inverse symbolic calculator:
   http://www.cecm.sfu.ca/projects/ISC

8. The CECM RevEng tool (see also Item 7):

9. Richard Crandall’s integer computation software:
   http://www.perfsci.com

10. Richard Fateman’s online integration tool:
    http://torte.cs.berkeley.edu:8010/tiltu

11. The FFTW site (FFT software):
    http://www.fftw.org
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12. The FIZ-Karlsruhe journal and abstract database:
http://www.zblmath.fiz-karlsruhe.de

13. The GNU high-precision arithmetic library:
http://www.gnu.org/software/gmp/gmp.html

14. The LBNL double-double, quad-double, and arbitrary precision computation software:
http://www.experimentalmath.info

15. The LBNL Experimental Mathematician’s Toolkit:
http://www.experimentalmath.info

16. The LBNL PiSearch facility (searches for names or hex digit sequences in the first several billion binary digits of $\pi$):
http://pisearch.lbl.gov

17. The Magma computational algebra system:
http://magma.maths.usyd.edu.au/magma

18. The Netlib software repository (linear algebra and other math software):
http://www.netlib.org

19. Neil Sloane’s online dictionary of integer sequences:
http://www.research.att.com/~njas/sequences

Other Resources

1. Lee Borrell’s “Absolute Certainty?” site:
http://www.fortunecity.com/emachines/e11/86/certain.html

2. Jonathan Borwein’s $\pi$ pages:
http://www.cecm.sfu.ca/~jborwein/pi_cover.html

3. The CECM $\pi$ recital site (recites $\pi$ in numerous languages):
http://www.cecm.sfu.ca/pi/yapPong.html

4. Gregory Chaitin’s site on algorithmic information theory:
http://www.cs.umaine.edu/~chaitin

5. The de Smit-Lenstra site on the mathematics of Escher’s “Print Gallery”:
http://escherdroste.math.leidenuniv.nl

6. Stewart Dickson’s math art site:
http://emsh.calarts.edu/~mathart
7. The electronic geometry site:
   http://www.eg-models.de
8. The Embree-Trefethen-Wright pseudospectra and eigenproblem site:
   http://web.comlab.ox.ac.uk/projects/pseudospectra
9. Helaman Ferguson’s mathematical sculpture site:
   http://www.helasculpt.com
10. Steven Finch’s mathematical constant site:
    http://pauillac.inria.fr/algo/bsolve/constant/constant.html
11. The Geometry Analysis Numerics Graphics (GANG) site:
    http://www.gang.umass.edu
12. Xavier Gourdon and Pascal Sebah’s site for famous math constants:
    http://numbers.computation.free.fr/Constants/constants.html
13. Andrew Granville’s Pascal triangle site:
    http://www.cecm.sfu.ca/organics/papers/granville/support/pascalform.html
14. David Griffeath’s cellular automata site:
    http://psoup.math.wisc.edu
15. Jerry Grossman’s Erdős number site:
    http://www.oakland.edu/enp/
16. Thomas Hales’ Kepler problem site:
    http://www.math.pitt.edu/~thales/kepler98
17. David Joyce’s site (Java implementation of Euclid’s Elements, and
    the Mandelbrot and Julia set explorer):
    http://aleph0.clarku.edu/~djoyce
18. Yasumasa Kanada’s π site:
    http://www.super-computing.org
19. Donald Knuth’s site on primes in π:
    http://mathpages.com/home/kmath184/kmath184.htm
20. The Mersenne prime site:
    http://www.mersenne.org
21. National Institute of Standards and Technology’s Digital Library of
    Mathematical Functions:
    http://dlmf.nist.gov
22. The Organic Mathematics Project site:  
   http://www.cecm.sfu.ca/organics

23. The Piworld site (features artwork based on π):  
   http://www.piworld.de

24. George Reese’s Buffon needle site:  
   http://www.mste.uiuc.edu/reese/buffon/buffon.html

25. RSA Security’s factorization challenge site:  
   http://www.rsasecurity.com/rsalabs/node.asp?id=2094

26. Saint Andrews College’s history of mathematics site (and curve resource):  
   http://www-gap.dcs.st-and.ac.uk/~history

27. Rob Scharein’s KnotPlot research and development site:  
   http://www.colab.sfu.ca/KnotPlot

28. Angela Vierling’s mathematical models site:  
   http://math.bu.edu/people/angelav/projects/models

29. Jeff Weeks’ topology and geometry site:  
   http://www.geometrygames.org

30. Figure 1.7 shows a Sierpinski cube plotted in JavaView  

Figure 1.7. The Sierpinski cube.
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1.9 Commentary and Additional Examples

1. **The old and the new.** David Joyce’s Java implementation of Euclid’s *Elements* and his *Mandelbrot and Julia Set Explorer* show what technology can offer, for old and new material, when used appropriately:

   [http://aleph0.clarku.edu/~djoyce/java/elements/elements.html](http://aleph0.clarku.edu/~djoyce/java/elements/elements.html) and [http://aleph0.clarku.edu/~djoyce/julia/explorer.html](http://aleph0.clarku.edu/~djoyce/julia/explorer.html)

2. **Dedekind’s preference for mental constructs** is also apparent in his development of the real numbers [84]:

   Many authors who adopted Dedekind’s basic ideas preferred not to follow him in defining the real numbers as creations of the mind corresponding to cuts in the system of rational numbers. ... Bertrand Russell emphasised the advantage of defining the real numbers simply as ... segments of the rationals. ... But Dedekind had his reasons ... for defining the real numbers as he did. When Heinrich Weber expressed his opinion in a letter to Dedekind that an irrational number should be taken to be the cut, instead of something new which is created in the mind and supposed to correspond to the cut, Dedekind replied “We have the right to grant ourselves such a creative power, and besides it is much more appropriate to proceed thus because of the similarity of all numbers. The rational numbers surely also produce cuts, but I will certainly not give out the rational number as identical with the cut generated by it; and also by introduction of the irrational numbers, one will often speak of cut-phenomena with such expressions, granting them such attributes, which applied to the numbers themselves would sound quite strange.” [103] page 224

3. **Hardy’s “apology.”** G. H. Hardy (1877–1947), the leading British analyst of the first half of the 20th century, wrote compellingly in defense of pure mathematics. In his essay, *A Mathematician’s Apology* [107], he noted that

   All physicists and a good many quite respectable mathematicians are contemptuous about proof.

   Hardy’s *Apology* is also a spirited defense of beauty over utility:

   Beauty is the first test. There is no permanent place in the world for ugly mathematics.
Along this line, many have noted his quote, 

Real mathematics . . . is almost wholly “useless.”

This has been overplayed and is now very dated, given the importance of cryptography, data compression and other applications of algebra and number theory that have arisen in recent years. But Hardy does acknowledge that if number theory could be employed for any “practical and obviously honourable purpose,” then “neither Gauss nor any other mathematician would have been so foolish as to decry or regret such applications.”

4. **Ramsey’s theorem.** Ramsey’s theorem asserts that given positive integers \(k\) and \(l\) there is an integer \(R(k, l)\) so that any graph with \(R(k, l)\) vertices either possesses a clique (complete subgraph) with \(k\) vertices or an independent set with \(l\) vertices. \(R(3) = R(3, 3) = 6\) and \(R(4) = R(4, 4) = 18\). This is often described as saying that at a six-person dinner party either there are three friends or there are three strangers. Such numbers \(R(k, 1)\) are very hard to compute.

Indeed, Paul Erdős suggested that if an alien demanded we give it the value of \(R(5)\) in order to save the Earth, we should set all mathematicians and computers to calculating the value. But if the alien demanded \(R(6)\), then humanity should attempt to destroy it before it destroyed us.

The following is from the site: [http://www.math.uchicago.edu/~mileti/museum/ramsey.html](http://www.math.uchicago.edu/~mileti/museum/ramsey.html)

One version of Ramsey’s Theorem states that no matter which number \(k\) you choose, you can find a number \(n\) such that given any arrangement of \(n\) pegs, [connected by red or green string] there must exist a monochromatic collection of \(k\) pegs. We will denote the smallest such \(n\) that works for a given \(k\) by \(R(k)\). The above results can be stated more succinctly by saying that \(R(3) = 6\) and \(R(4) = 18\). It is easy to see that \(R(1) = 1\) (given only 1 peg, there are no pieces of string, so it forms a monochromatic collection for vacuous reasons) and \(R(2) = 2\) (If you only have 2 pegs, there is only piece of string, so the 2 pegs form a monochromatic collection).

Perhaps surprisingly, nobody knows the value of \(R(k)\) for any \(k\) larger than 4. The best results currently known state that \(R(5)\) is somewhere between 43 and 49 (inclusive) and \(R(6)\) is somewhere between 102 and 165. You might wonder why, given the incredible computing power at our disposal, we can not simply
search through all arrangements of string for 43 pegs through 49 pegs to find the actual value of $R(5)$. However, one can calculate that there are $2^{903}$ (a number that has 272 decimal digits!) ways to arrange red and green string among 43 pegs, which is a number beyond ordinary comprehension (scientists estimate that there are about 80 digits in the number of electrons in the universe). By using symmetry, one can drastically lower the number of such arrangements a computer would have to look at, but even if we only had to examine 1 out of every 1 trillion configurations, we would still be left with over $2^{864}$ arrangements (a number that has 261 digits!). Estimating the values of $R(k)$ requires mathematical ingenuity in addition to brute force calculations.

5. **Gödel’s theorem and complexity.** While there are still no “ordinary” Gödel statements (that is, true but unprovable), the Paris-Harrington theorem comes close. It is “[a]n arithmetically expressible true statement from finitary combinatorics... that is not provable in Peano arithmetic. The statement $S$ in question is the strengthening of the finite Ramsey theorem by requiring the homogeneous set $H$ to be ‘relatively large,’ i.e., card $H \geq \min H$.” (Math Reviews). See also [http://www.cs.utexas.edu/users/moore/best-ideas/nqthm](http://www.cs.utexas.edu/users/moore/best-ideas/nqthm) and [http://www.fortunecity.com/emachines/e11/86/certain.html](http://www.fortunecity.com/emachines/e11/86/certain.html).

6. **Goodstein’s theorem.** Another very striking example is that of Goodstein sequences [131]. Consider writing a number base $b$. Doing the same for each of the exponents in the resulting representations, until the process stops, yields the hereditary base $b$ representation of $n$. For example, the hereditary base 2 representation of 266 is

$$266 = 2^{2^{2+1}} + 2^{2+1} + 2^1.$$  

**Base change.** Let $B_b(n)$ be the natural number obtained on replacing each $b$ by $b+1$ in the hereditary base $b$ representation of $n$. For example, “bumping the base” from 2 to 3 above gives

$$B_2(266) = 3^{3^{3+1}} + 3^{3+1} + 3.$$  

Consider a sequence of integers obtained by repeatedly applying the operation: **Bump the base and subtract one from the result.** Iteratively performing this procedure for 266 yields
Done generally, this determines the Goodstein sequence starting at \( n \).
That is, we recursively define nonnegative integers \( n_0 = n, n_1, \cdots, n_k, \cdots \) by
\[
n_{k+1} = B_{k+2}(n_k) - 1,
\]
if \( n_k > 0 \) and \( n_{k+1} = 0 \) otherwise. We initially obtain very rapid growth: \( 266_8 \approx 10^{10^{11}} \) and \( 4_k \) first reaches 0 for \( k = 3 \) \( (2^{402653211} - 1) \approx 10^{121210695} \).

However, Goodstein in 1944 proved that every Goodstein sequence converges to 0.

Remarkably, in 1982 Paris and Kirby showed that Goodstein’s theorem is not provable in ordinary Peano arithmetic, despite being a fairly ordinary sounding number-theoretic fact.

There are quite natural, closely related games on finite trees such as “Hercules and the Hydra” in which the fact that Hercules always has a winning strategy to defeat a many-headed hydra is independent of arithmetic. Such results show that even in a seemingly computational framework, we may bump into Gödel’s theorem \[131\].

7. Hales’ computer-assisted proof of Kepler’s conjecture. In 1611, Kepler described the stacking of equal-sized spheres into the familiar arrangement we see for oranges in the grocery store. He asserted that this packing is the tightest possible. This assertion is now known as the Kepler conjecture, and has persisted for centuries without rigorous proof. Hilbert included the Kepler conjecture in his famous list of unsolved problems in 1900. In 1994, Thomas Hales, now at the University of Pittsburgh, proposed a five-step program that would result in a proof: (a) treat maps that only have triangular faces; (b) show that the face-centered cubic and hexagonal-close packings are local maxima in the strong sense that they have a higher score than any Delaunay star with the same graph; (c) treat maps that
1. What is Experimental Mathematics?

contain only triangular and quadrilateral faces (except the pentagonal prism); (d) treat maps that contain something other than a triangle or quadrilateral face; (e) treat pentagonal prisms.

In 1998, Hales announced that the program was now complete, with Samuel Ferguson (son of Helaman Ferguson) completing the crucial fifth step. This project involved extensive computation, using an interval arithmetic package, a graph generator, and Mathematica. The computer files containing the source code and computational results occupy more than three Gbytes of disk space. Additional details, including papers, are available at the URL [http://www.math.pitt.edu/~thales/kepler98](http://www.math.pitt.edu/~thales/kepler98).

As this book was going to press, the *Annals of Mathematics* has decided to publish Hales’ paper, but with a cautionary note, because although a team of referees is “99% certain” that the computer-assisted proof is sound, they have not been able to verify every detail [186]. One wonders if every other article in this journal has implicitly been certified to be correct with more than 99% certainty.


1. Counting sheep
   When you’re trying to sleep,
   Being fair
   When there’s something to share,
   Being neat
   When you’re folding a sheet,
   That’s mathematics!

2. When a ball
   Bounces off of a wall,
   When you cook
   From a recipe book,
   When you know
   How much money you owe,
   That’s mathematics!

3. How much gold can you hold in an elephant’s ear?
   When it’s noon on the moon,
   then what time is it here?
   If you could count for a year,
   would you get to infinity,
   Or somewhere in that vicinity?

4. When you choose
   How much postage to use,
   When you know
   What’s the chance it will snow,
   When you bet
   And you end up in debt,
   Oh try as you may,
   You just can’t get away
   From mathematics!
5. Andrew Wiles gently smiles, Does his thing, and voila! Q.E.D., we agree, And we all shout hurrah! As he confirms what Fermat Jotted down in that margin, Which could’ve used some enlargin’. Yes, try as you may, You just can’t get away From mathematics!

6. Tap your feet, Keepin’ time to a beat Of a song While you’re singing along, Harmonize With the rest of the guys, Yes, try as you may, You just can’t get away From mathematics!

9. Mathematics of Escher’s “Print Galley.” In Maurits C. Escher’s 1956 painting “Prentententoonstelling,” a young man is viewing a painting in an exhibition gallery. As his eyes follow the waterfront buildings shown in this painting around in a circle, he discovers among these buildings the very gallery he is standing in. Bart de Smit and Hendrik Lenstra have shown that the painting can be viewed as drawn on an elliptic curve over the complex plane, and if continued would repeat itself, with each iteration reduced in size by a factor of $22.5836845286\ldots$ and rotated clockwise by $157.625560832\ldots$ degrees $[82]$. This research received feature coverage in the New York Times [173]. Details are available at the URL [http://escherdroste.math.leidenuniv.nl].

10. Techniques for putting the Internet to work.

As a teenager in early 19th Century Britain, Michael Faraday struggled to overcome a lack of formal education by reading (among other things) self-help books that were popular at the time. It was from one such book (Improvement of the Mind, authored by Isaac Watts) that Faraday learned four ways to become smarter: (1) attend lectures, (2) take notes, (3) correspond with people of similar interests, (4) join a discussion group. (Scott Butner, ChemAlliance Staff)


The article starts by quoting Arthur C. Clarke: “Any sufficiently advanced technology is indistinguishable from magic.” Until Minovitch discovered that the so-called Hohmann transfer ellipses were not the
minimum energy way of getting to the outer planets, “most planetary mission designers considered the gravity field of a target planet to be somewhat of a nuisance, to be cancelled out, usually by onboard Rocket thrust.” For example, without a gravitational boost from the orbits of Saturn, Jupiter and Uranus, the Earth-to-Neptune Voyager mission (achieved in 1989 in little more than a decade) would have taken more than 30 years!

12. **John Maynard Keynes.** Two excerpts follow from *Keynes the Man*, written on the 50th anniversary of the great economist’s death, by Sir Alec Cairncross, in the *Economist*, April 20, 1996:

> Keynes distrusted intellectual rigour of the Ricardian type as likely to get in the way of original thinking and saw that it was not uncommon to hit on a valid conclusion before finding a logical path to it. . . . “I don’t really start,” he said, “until I get my proofs back from the printer. Then I can begin serious writing.”

Keynes’ undergraduate training was in mathematics at Cambridge, where he excelled as at most things he tried. He was an avid collector of rare books and manuscripts, Newton’s included. Keynes and Hardy were virtually the only scientists who intersected with the Bloomsbury group.

13. **A world of doughnuts and spheres.** As this book was going to press, the Russian mathematician Grigori Perelman was lecturing on a proof of the *Poincaré Conjecture*. His potentially ground-breaking work, if found to be valid, may earn him a share of a $1 million prize for solving one of the Clay Mathematics Institute’s “Millennium Prize Problems.” The Clay Institute’s web site describes the Poincaré Conjecture in these terms:

> If we stretch a rubber band around the surface of an apple, then we can shrink it down to a point by moving it slowly, without tearing it and without allowing it to leave the surface. On the other hand, if we imagine that the same rubber band has somehow been stretched in the appropriate direction around a doughnut, then there is no way of shrinking it to a point without breaking either the rubber band or the doughnut [Figure 1.8]. We say the surface of the apple is “simply connected,” but that the surface of the doughnut is not. Poincaré, almost a hundred years ago, knew that a two dimensional sphere is essentially characterized by this property of simple connectivity, and asked the corresponding question for the three dimensional sphere (the
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Peter Sarnak, a well-known Princeton University mathematician, described Perelman’s work in these words: “He’s not facing Poincaré directly, he’s just trying to do [a] grander scheme.” The Poincaré result is merely “a million dollar afterthought.” Prof. Sun-Yung Alice Chang observed that the Poincaré Conjecture is “in the same scale as Fermat’s Last Theorem. [Proving] it puts you in the history of mathematics; the dream of every mathematician” \[64\]. Along this line, a \textit{New York Times} report \[122\] observed, “That grown men and women can make a living pondering such matters is a sign that civilization, as fragile as it may sometimes seem, remains intact.”

14. The number partitioning problem. Given a set of $n$ nonnegative integers $a_1, a_2, \ldots, a_n$, the number partitioning problem is to divide this set into two subsets such that the sums of the numbers in each subset are as nearly equal as possible. Brian Hayes calls this “the easiest hard problem” \[111\]. It is well known to be $NP$-complete. Nonetheless, some reasonably effective heuristic algorithms are known for solution. Hayes provides the following analogy for one of these:

One of the cherished customs of childhood is choosing up sides for a ball game. Where I grew up, we did it this way: The two chief bullies of the neighborhood would appoint themselves captains of the opposing teams, and then they would take turns picking other players. On each round, a captain would choose the most capable (or, toward the end, the least inept) player from the pool of remaining candidates, until everyone present had been assigned to one side or the other. The aim of this ritual was to produce two evenly matched teams and, along the way, to remind each of us of our precise ranking in the neighborhood pecking order. It usually worked.
None of us in those days—not the hopefuls waiting for our name to be called, and certainly not the two thick-necked team leaders—recognized that our scheme for choosing sides implements a greedy heuristic for the balanced number partitioning problem. And we had no idea that this problem is NP-complete—that finding the optimum team rosters is certifiably hard. We just wanted to get on with the game.

Solutions to this problem exhibit a curious experimental phenomenon: When $n$ is smaller than the number of bits needed to encode the $a_i$, the computational cost grows exponentially with $n$. When $n$ is larger than this value, the computational cost actually decreases, then levels off, growing only linearly with $n$ [154].

15. Hersh’s humanist philosophy of mathematics. However hard mathematical paradigm shifts are to accept and whatever the result of these tides, mathematics is and will remain a uniquely human undertaking. Indeed, Reuben Hersh’s arguments for a humanist philosophy of mathematics [113, 114], as paraphrased below, become even more convincing in our experimental setting:

1. Mathematics is human. It is part of and fits into human culture. It does not match Frege’s concept of an abstract, timeless, tenseless, objective reality.

2. Mathematical knowledge is fallible. As in science, mathematics can advance by making mistakes and then correcting or even re-correcting them. The “fallibilism” of mathematics is brilliantly argued in Lakatos’ Proofs and Refutations.

3. There are different versions of proof or rigor. Standards of rigor can vary depending on time, place, and other things. The use of computers in formal proofs, exemplified by the computer-assisted proof of the four color theorem in 1977, is just one example of an emerging nontraditional standard of rigor.

4. Empirical evidence, numerical experimentation and probabilistic proof all can help us decide what to believe in mathematics. Aristotelian logic isn’t necessarily always the best way of deciding.

5. Mathematical objects are a special variety of a social-cultural-historical object. Contrary to the assertions of certain postmodern detractors, mathematics cannot be dismissed as merely a new form of literature or religion. Nevertheless, many mathematical objects can be seen as shared ideas, like Moby Dick in literature, or the Immaculate Conception in religion.
16. **Quantum Computer, n.** a radical, still largely theoretical, alternative to the von Neuman architecture of present digital computers. First posited by Richard Feynman in 1982, and detailed by Deutsch (1985) it relies on exploiting quantum mechanical properties of: quantization, entanglement, and especially quantum interference. Interference means outcomes of quantum processes depend on all possible histories of a process, and makes quantum computers exponentially more powerful than classical ones. Entanglement means spatially separated, non-interacting, systems with prior interaction may still have locally inaccessible information in common. This is what makes quantum encryption possible. The field exploded after 1994 when Peter Shor discovered a quantum algorithm for efficient factorization of very large numbers. Such methods would render current coding theory and encryption techniques, such as RSA, ineffective.

**qubit, n.** the quantum computer analogue of a computer bit. It models the fact that atoms can be prepared in a superposition of two different electronic states. Analogously, a quantum two-state system—a quantum bit or qubit—can be prepared in a superposition of its two logical states 0 and 1. Thus a qubit can simultaneously be both 0 and 1. (The above two definitions are taken from [41].)

17. Mathematics, history and philosophy.

The history of mathematics, lacking the guidance of philosophy, has become blind, while the philosophy of mathematics, turning its back on the most intriguing phenomena in the history of mathematics, has become empty. (Imre Lakatos, in *Proofs and Refutations* [138, 124])

18. **Nature of mathematical genius.** Mathematical genius appears to be a rare but remarkable phenomenon. Is it a genetic? An emergent accident of DNA? The result of good parenting? A stimulating intellectual environment? The product of inspiring teachers?

(a) Recent interviews (Peter Liljedahl, SFU, unpublished PhD work) with top-level mathematicians suggests that most do not read very much, preferring to have results described to them, and put a large emphasis on the role of chance—which always favors the prepared mind.
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(b) Mathematical genius is almost always noted early in life and blossoms rather soon. As G. H. Hardy observed in his *A Mathematician’s Apology*, “Mathematics, more than any other art or science, is a young man’s game. . . . I do not know an instance of a major mathematical advance initiated by a man past fifty. . . . [Newton’s] “greatest ideas of all, fluxions and the law of gravitation, came to him about 1666, when he was twenty-four.” [107, pg. 78]. Needless to say, this does not bode well for the present authors!

(c) Archimedes, Newton, Euler, Gauss, Ramanujan, and others all seem to have had extraordinary facilities for numerical and algebraic computation. Most of us know the story of Gauss who, when his teacher asked the class to sum the integers from 1 to 100, quickly noted that this was $50 \times 101 = 5050$, and was the only student to obtain the correct answer! Ramanujan’s genius was his incredible skill at algebraic manipulation, a skill that flowered largely in a vacuum of advanced training in modern mathematics. The following is told of John von Neumann, who made fundamental contributions to computer science, mathematical economics, meteorology, probability theory, and quantum mechanics in the early 20th century [139, pg. 10]:

Two bicyclists are 20 miles apart and head toward each other at 10 miles per hour each. At the same time a fly traveling at a steady 15 miles per hour starts from the front wheel of the northbound bicycle. It lands on the front wheel of the southbound bicycle, and then instantly turns around and flies back, and after next landing instantly flies north again. Question: What total distance did the fly cover before it was crushed between the two front wheels?

The slow way of answering is to calculate the distance that the fly travels on its first trip to the southbound front wheel, then the distance it travels on its next trip to the northbound wheel, and finally to sum the infinite series so obtained. . . . The short way is to note that the bicycles will meet exactly an hour after starting, by which time the 15-miles-per-hour fly must have covered 15 miles. When the question was put to [John von Neumann], he danced and answered immediately, “15 miles.” “Oh, you’ve heard the trick before,” said the disappointed questioner. “What trick?” asked the puzzled Johnny. “I simply summed the infinite series.”
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(d) Others are known for their prodigious skill and boundless energy in ranging over a wide variety of very difficult topics with ease. The following is told of Nobel-prize-winning mathematical physicist Richard Feynman, during a lecture at CalTech [97 145]:

Feynman immediately rose, astonishingly, to say that such objects would be gravitationally unstable. Furthermore, he said that the instability followed from general relativity. The claim required a calculation of the subtle countervailing effects of stellar forces and relativistic gravity. Fowler thought he was talking through his hat. A colleague later discovered that Feynman had done a hundred pages of work on the problem years before. The Chicago astrophysicist Subrahmanyan Chandrasekhar independently produced Feynman’s result—it was part of the work for which he won a Nobel Prize twenty years later. Feynman himself never bothered to publish. Someone with a new idea always risked finding, as one colleague said, “that Feynman had signed the guest book and already left.”

John Maynard Keynes, who studied the original writings of Isaac Newton while riding taxicabs between British treasury board meetings, wrote this of Newton on the tricentenary of his birth [128 145]:

His peculiar gift was the power of holding continuously in his mind a purely mental problem until he had seen straight through it. I fancy his pre-eminence is due to his muscles of intuition being the strongest and most enduring with which a man has ever been gifted. Anyone who has ever attempted pure scientific or philosophical thought knows how one can hold a problem momentarily in one’s mind and apply all one’s powers of concentration to piercing through it, and how it will dissolve and escape and you find that what you are surveying is a blank. I believe that Newton could hold a problem in his mind for hours and days and weeks until it surrendered to him its secret. Then being a supreme mathematical technician he could dress it up, how you will, for purposes of exposition, but it was his intuition which was pre-eminently extraordinary—“so happy in his conjectures,” said de Morgan, “as to seem to know more than he could possibly have any means of proving.”

(e) In a recent provocative essay, David Lykken explores the emergence of genius. Here is his conclusion [145]:

Ericsson and Charness [89] are willing to acknowledge that genetic differences in temperament and “preferred activity
level” may determine which of us go for the gold but, curiously, they cling to the assumption that individual genetic differences in both physical and mental capacities are not important, perhaps nonexistent. This would require us to believe that … little Gauss’s ability to correct his father’s arithmetic at three and confound his school master at ten resulted, not from extraordinary mental hardware, but from mental software acquired through self-directed practice in an intellectually unstimulating environment.

Those of us who have studied MZ [monozygote, i.e., identical] twins reared apart from one another find these assumptions … incredible. We cannot believe that MZA twins [monozygote twins reared apart] correlate .75 in IQ merely because, in their separate environments, their similarities in temperament led them to indulge in very similar amounts of practice on very similar topics. …

I think we must agree with Ericsson, however, that works of genius tend to be the product of minds enriched by years of concentrated effort. Isaac Newton often became so caught up in cerebration that he would forget to eat or sleep. Edwin Land, inventor of the instant Polaroid camera and of a sophisticated computational theory of color vision, sometimes worked at his desk for 36 hours or more, unaware of the passage of time until he felt faint on standing up. Similar stories were told of Edison. It does not follow, however, that these were ordinary minds to begin with.

Edison, Feynman, Land, and Newton all from their boyhood had intense curiosity, an enthusiasm or zeal for discovery and understanding. Each of them was able to take seriously hypotheses that others thought to be implausible (or had not thought about at all). All four possessed a kind of intellectual arrogance that permitted them to essay prodigious tasks, to undertake to solve problems that most of their contemporaries believed to be impossible. And each of them had quite extraordinary powers of concentration. …

I think what lies at the heart of these mysteries is genetic, probably emergenic. The configuration of traits of intellect, mental energy, and temperament with which, during the plague years of 1665–6, Isaac Newton revolutionized the world of science were, I believe, the consequence of a genetic lottery that occurred about nine months prior to his birth, on Christmas day, in 1642.
Experimental Mathematics in Action

The purpose of computing is insight, not numbers.

In this chapter, we will present a few particularly engaging examples of modern experimental mathematics in action. We invite those readers with access to some of the computational tools we mention below to personally try some of these examples—with some sense of realism.

2.1 Pascal’s Triangle

Although Blaise Pascal (1623–1662) is commonly credited with what is now known as Pascal’s triangle (namely the array of integers such that row \( m \) and column \( n \) has the value

\[
\binom{m}{n} = \frac{m!}{n!(m-n)!},
\]

(2.1)

this well-known numerical scheme is actually much older. The earliest written account may be in a 1303 Chinese book by Chu Shih-Chieh, entitled *Precious Mirror of the Four Elements*, but even here, Pascal’s triangle is called “The Old Method.” Thus it is at least 700 years old, and probably centuries older still. Given its simplicity and antiquity, it is natural to expect that every conceivable aspect of this venerable scheme has been discovered and studied at length. But even in such arenas, diligent researchers can sometimes glean new insights.

Start with the familiar binomial coefficient,

\[
\binom{m}{n} = \frac{m!}{n!(m-n)!},
\]

and consider the remainders on division by 2. That is, set

\[
F_2(m, n) = \binom{m}{n} \mod 2.
\]

(2.2)
Let $N_2(m)$ be the number of 1s in the set $(F_2(m, n), 0 \leq n \leq m)$.

By means of an algebraic argument, it can be shown that $N_2(m)$ is given by

$$N_2(m) = 2^{B_1(m)}, \quad (2.3)$$

where $B_1(m)$ is the number of 1s in the binary representation of $m$ \[101].

But there is another proof of this fact that demonstrates the power of visualization in experimental mathematics.

Pascal’s triangle has long been used as a tool to visualize the behavior of the binomial coefficient function. For example, the combinatorial identity

$$\binom{m}{n} = \binom{m-1}{n-1} + \binom{m-1}{n}$$

is equivalent to the Pascal triangle rule that the value of entry $(m, n)$ is merely the sum of the entries to the left and right of it, on the previous row. As another example, the fact that binomial coefficients are greatest when $n = \lfloor m/2 \rfloor$ is evident from visual inspection—centrally located cells have had the greatest benefit of the combining add operation in the rows above, and this visual observation can indeed be fashioned into a rigorous proof.

Consider now a modified Pascal triangle where entries are reduced modulo 2, as shown in Figure 2.1. Such a figure was easy to generate using the Internet-based tool available at [http://www.cecm.sfu.ca/organics/papers/granville/support/pascalform.html](http://www.cecm.sfu.ca/organics/papers/granville/support/pascalform.html). It is evident from the left-hand image in Figure 2.1 (see Color Plate I), which comes from the interface, that the entries of this Pascal triangle form a Sierpinski triangle, which in the limit is a self-similar figure akin to those studied by Mandelbrot [151]. In fact, it can be seen that this figure exhibits the fractional dimension

$$\log_2 3 = 1.58496 \ldots$$

The right-hand figure shows a computer realization of this process on a tetrahedron, due to Darrell Hepting. Now let’s take a look at a proof of identity (2.3) in the style of experimental mathematics, a proof that we argue is significantly easier than the usual algebraic proof of this result.

Given a positive integer $m$, construct a Pascal triangle modulo 2 of size $2^\lceil \log_2 m \rceil$. In this way the $m$-th row corresponds to a line that crosses the lower half of the largest upright triangle. Note that successive binary digits of $m$ specify whether the line crosses the upper (0) or the lower (1) half of successively smaller upright triangles. The upper halves always contain one half-sized upright triangle, whereas the lower halves contain two such triangles. The total number of triangles crossed by the line is thus multiplied by a factor of two whenever the lower half is crossed. The total number of ones in the $m$-th row is thus the product of the factors of two
2.1. Pascal’s Triangle

Figure 2.1. Pascal triangles modulo two? (see Color Plate I.) Courtesy of Daryl Hepting.

associated with each one in the binary expansion of \( m \). This proves (2.3). See Stephen Wolfram’s article [193] and the Crandall-Pomerance book [77] (research problem 8.22) for additional details and some generalizations.

We should add here that Wolfram has recently published his long-awaited tome \textit{A New Kind of Science}, an exhaustive study of cellular automata with connections to numerous other fields of science. Wolfram’s approach in this book is almost exclusively experimental, employing nearly 1000 high-resolution graphical examples to highlight his observations, building up to his “Principle of Computational Equivalence.” In this regard, one could view Pascal’s triangle modulo 2 as merely a particular instance of a one-dimensional cellular automata [194].

We might note in passing that the Sierpinski triangle has a habit of appearing in quite a few unexpected places in mathematics. One remarkable example, in quite a different context, is the following. Construct an “arbitrary” triangle, with vertices \((x_1, y_1), (x_2, y_2)\) and \((x_3, y_3)\). Specify a starting point \((x, y)\) within the triangle. Then iterate the following construction: First select a random integer \( r \) in the set \((1, 2, 3)\), and then construct a new point \((x', y')\) as follows:

\[
(x', y') = \left( \frac{1}{2}(x + x_r), \frac{1}{2}(y + y_r) \right).
\]  

(2.4)

This procedure is then iterated indefinitely.
If you carry out this procedure on a computer with a high-resolution display, it is immediately evident that, no matter what triangle is specified, and no matter what initial point is selected, the resulting figure (after possibly the first few points) is a Sierpinski triangle contained in the original triangle—see, for example, Figure 2.2. In other words, the Sierpinski triangle is the “attractor” set for this iteration (by the way, it is easier to “see” this fact than to prove it). The study of these fractal objects and the schemes used to generate them is by itself a fascinating example of experimental mathematics in action. See, for example, Michael Barnsley’s interesting book, Fractals Everywhere [30].

2.2 A Curious Anomaly in the Gregory Series

In 1988, Joseph Roy North of Colorado Springs observed that Gregory’s series for $\pi$, 

![Sierpinski triangle by random selections.](image)

Figure 2.2. Sierpinski triangle by random selections.
2.2. A Curious Anomaly in the Gregory Series

\[
\pi = 4 \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{2k-1} = 4(1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots), \tag{2.5}
\]

when truncated to 5,000,000 terms, gives a value that differs strangely from the true value of \(\pi\). Here is the truncated Gregory value and the true value of \(\pi\):

\[
\begin{align*}
\text{Truncated Gregory value:} & \quad 3.14159265358979323846264338327950288419716939937510582097494459230781640... \\
\text{True value of } \pi & \quad 3.14159265358979323846264338327950288419716939937510582097494459230781640...
\end{align*}
\]

The series value differs, as one might expect from a series truncated to 5,000,000 terms, in the seventh decimal place—a “4” where there should be a “6.” But the next 13 digits are correct! Then, following another erroneous digit, the sequence is once again correct for an additional 12 digits. In fact, of the first 46 digits, only four differ from the corresponding decimal digits of \(\pi\). Further, the “error” digits appear to occur in positions that have a period of 14, as shown above. Such anomalous behavior begs explanation.

Once observed, it is natural (and easy given a modern computer algebra system) to ask if something similar happens with the logarithm. Indeed it does, as the following value obtained by truncating the series \(\log 2 = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \cdots\) shows:

\[
\begin{align*}
\text{Truncated logarithm value:} & \quad 0.6931471805599453094172321\ldots \\
\text{True value of } \log 2 & \quad 0.6931471805599453094172321\ldots
\end{align*}
\]

Here again, the “erroneous” digits appear in locations with a period of 14. In the first case, the differences from the “correct” values are (2, -2, 10, -122, 2770), while in the second case the differences are (1, -1, 2, -16, 272, -7936). We note that each integer in the first set is even; dividing by two, we obtain (1, -1, 2, -16, 1385).

How can we find out exactly what is going on here? A great place to start is by enlisting the help of an excellent resource for the computational mathematician: Neil Sloane and Simon Plouffe’s Internet-based integer sequence recognition tool, available at [http://www.research.att.com/~njas/sequences](http://www.research.att.com/~njas/sequences). This tool has no difficulty recognizing the first sequence as “Euler numbers” and the second as “tangent numbers.” Euler numbers and tangent numbers are defined in terms of the Taylor’s series for \(\sec x\).
and \( \tan x \), respectively:

\[
\sec x = \sum_{k=0}^{\infty} \frac{(-1)^k E_{2k} x^{2k}}{(2k)!}
\]

\[
\tan x = \sum_{k=0}^{\infty} \frac{(-1)^{k+1} T_{2k+1} x^{2k+1}}{(2k + 1)!}.
\]

Indeed, this discovery, made originally through the print version of the sequence recognition tool available more than a decade ago, led to a formal proof that these sequences are indeed the source of the “errors” in these sequences. The precise result is that the following asymptotic expansions hold:

\[
\frac{\pi}{2} - 2 \sum_{k=1}^{N/2} \frac{(-1)^{k+1} 2k - 1}{E_{2m}} \approx \sum_{m=0}^{\infty} \frac{E_{2m}}{N^{2m+1}}
\]

\[
\log 2 - \sum_{k=1}^{N/2} \frac{(-1)^{k+1}}{k} \approx \frac{1}{N} + \sum_{m=1}^{\infty} \frac{T_{2m-1}}{N^{2m}}.
\]

Now the genesis of the anomaly mentioned above is clear: North, in computing \( \pi \) by Gregory’s series, had by chance truncated the series at 5,000,000 terms, which is exactly one-half of a fairly large power of ten. Indeed, setting \( N = 10,000,000 \) in Equation (2.7) shows that the first hundred or so digits of the truncated series value are small perturbations of the correct decimal expansion for \( \pi \). And the asymptotic expansions show up on the computer screen, as we observed above. Similar phenomena occur for other constants. (See [46] for proofs of (2.7) and (2.8), together with some additional details.)

### 2.3 Bifurcation Points in the Logistic Iteration

Of course, our earlier remarks about pure mathematicians being slow to take advantage of the computer do have some exceptions. In particular, the entire area of dynamical systems (sometimes referred to as chaos theory) owes its very existence to modern information technology. And one of the classic examples of a chaotic iteration is known as the logistic iteration: Fix a real number \( r > 0 \), select \( x_0 \) in the unit interval \((0, 1)\), and then iterate

\[
x_{k+1} = rx_k(1 - x_k).
\]

(2.9)
This is termed the “logistic” iteration because of its roots in computational ecology: It mimics the behavior of a biological population, which, if it becomes too numerous, exhausts its available food supply and then falls back to a smaller population, possibly oscillating in an irregular manner over many generations.

For values of $r < 1$, the iterates $(x_k)$ quickly converge to zero. For $1 < r < 3$, the iterates converge to a single nonzero limit point. At $r = 3$, a bifurcation occurs: For $3 < r < 3.449489 \ldots = 1 + \sqrt{6}$, the iterates oscillate between two distinct limit points. A second bifurcation occurs at $r = 1 + \sqrt{6}$. In particular, for $1 + \sqrt{6} < r < 3.544090359 \ldots$, the iterates oscillate in a periodic fashion between four distinct limit points. This pattern of limit point bifurcation and period doubling occurs at successively shorter intervals, until $r > 3.5699457 \ldots$, when iterates behave in a completely chaotic manner. This behavior is shown in Figure 2.3.

Until recently, the identity of the third bifurcation point, namely the constant $b_3 = 3.544090359 \ldots$, was not known. It is fairly straightforward, by means of recursive substitutions of Equation (2.9), to demonstrate that this constant must be algebraic, but the bound on the degree of the integer
polynomial that \( b_3 \) satisfies is quite large and thus not very useful.

A tool that can be used in such situations is an integer relation algorithm. This is an algorithm which, when given \( n \) real numbers \((x_1, x_2, \cdots, x_n)\), returns integers \((a_1, a_2, \cdots, a_n)\), not all zero, such that \( a_1x_1 + a_2x_2 + \cdots + a_nx_n = 0 \) (if such a solution exists). Such computations must be done using very high precision arithmetic, or else the results are not numerically significant. At present the best algorithm for integer relation detection appears to be the “PSLQ” algorithm of mathematician-sculptor Helaman Ferguson \[92\ [15] [23], although the “LLL” algorithm is also often used. We will discuss integer relation detection in greater depth in Section 6.3.1.

For the time being we mention the Internet-based integer relation tool at \url{http://www.cecm.sfu.ca/projects/IntegerRelations} and the Experimental Mathematician’s Toolkit at \url{http://www.experimentalmath.info}.

One straightforward application of an integer relation tool is to recover the polynomial satisfied by an algebraic number. If you suspect that a constant \( \alpha \), whose numerical value can be calculated to high precision, is algebraic of degree \( n \), then you can test this conjecture by computing the \((n+1)\)-long vector \((1, \alpha, \alpha^2, \cdots, \alpha^n)\), and then using this vector as input to an integer relation calculation. If it finds a solution vector \((a_0, a_1, a_2, \cdots, a_n)\) with a sufficiently high degree of numerical accuracy, then you can be fairly confident that these integers are precisely the coefficients of the polynomial satisfied by \( \alpha \).

In the present example, where \( \alpha = b_3 \), a predecessor algorithm to PSLQ recovered the polynomial

\[
0 = 4913 + 2108t^2 - 604t^3 - 977t^4 + 8t^5 + 44t^6 + 392t^7 - 193t^8 - 40t^9 + 48t^{10} - 12t^{11} + t^{12}. \tag{2.10}
\]

You might like to try to rediscover this polynomial by using the Internet-based tool mentioned above. To do this requires a high-precision value of \( b_3 \). Its value correct to 120 decimal digits is:

\[
3.5440903595 5192285361 5965986604 8045405830 9984544457 3675457812 2530305842 9428588630 1225625856 6424891799 9626089927 7589974545
\]

If you do not wish to type this number in, you may find it by using Mathematica:

\[
\text{FindRoot}[4913 + 2108t^2 - 604t^3 - 977t^4 + 8t^5 + 44t^6 + 392t^7 - 193t^8 - 40t^9 + 48t^{10} - 12t^{11} + t^{12} == 0, \{t, 3.544\}, \text{WorkingPrecision} \rightarrow 125]
\]

or by using a similar command with the Experimental Mathematician’s Toolkit.
Recently, the fourth bifurcation point \( b_4 = 3.564407266095 \ldots \) was identified by a similar, but much more challenging, integer relation calculation. In particular, it was found that \( \alpha = -b_4(b_4 - 2) \) satisfies a certain integer polynomial of degree 120. The recovered coefficients descend monotonically from \( 257^{30} \approx 1.986 \times 10^{72} \) down to 1. This calculation required 10,000 decimal digit precision arithmetic, and more than one hour on 48 processors of a parallel computer system. Full details can be found in [23]. The relation produced was recently verified by Konstantinos Karamanos, using the Magma computer algebra system [152].

We add in passing that the limiting ratio of the intervals between successive bifurcation points in the logistic iteration is 4.669201609 \ldots This is known as Feigenbaum’s constant, named for Mitchell Feigenbaum who first observed, as a result of computational experiments, that this limiting ratio holds for a wide class of chaotic iterations, not just the logistic iteration. A fascinating account of this discovery is given in [96]. Researchers have subsequently made numerous attempts to recognize Feigenbaum’s constant as an algebraic number, or as a simple formula involving other well-known constants of mathematics, but these efforts have failed so far. An algorithm for calculating Feigenbaum’s constant to high precision is given in [59].

### 2.4 Experimental Mathematics and Sculpture

In the previous section, we mentioned the PSLQ algorithm, which was discovered in 1993 by Helaman Ferguson. This is certainly a signal accomplishment—for example, the PSLQ algorithm (with associated lattice reduction algorithms) was recently named one of ten “algorithms of the century” by *Computing in Science and Engineering* [15]. Nonetheless Ferguson is even more well-known for his numerous mathematics-inspired sculptures, which grace numerous research institutes in the United States. Photos and highly readable explanations of these sculptures can be seen in a lovely book written by his wife, Claire [91]. Together, the Fergusons recently won the 2002 Communications Award, bestowed by the Joint Policy Board of Mathematics. The citation for this award declares that the Fergusons “have dazzled the mathematical community and a far wider public with exquisite sculptures embodying mathematical ideas, along with artful and accessible essays and lectures elucidating the mathematical concepts.”

Ferguson notes that the PSLQ algorithm can be thought of as a \( n \)-dimension extension of the Euclidean algorithm, and is, like the Euclidean scheme, fundamentally a “subtractive” algorithm. As Ferguson explains, “It is also true that my sculptural form of expression is subtractive: I get
my mathematical forms by direct carving of stone." [168]

There is a remarkable and unanticipated connection between Ferguson’s PSLQ algorithm and at least one of Ferguson’s sculptures. It is known that the volumes of complements of certain knot figures (which volumes in $\mathbb{R}^3$ are infinite) are finite in hyperbolic space, and sometimes are given by certain explicit formulas. This is not true of all knots. Many of these hyperbolic complements of knots correspond to certain discrete quotient subgroups of matrix groups.

One of Ferguson’s sculptures, known as the “Eight-Fold Way,” is housed at the Mathematical Sciences Research Institute in Berkeley, California (see Figure 2.4 Color Plate IV, and Item 33 at the end of this chapter).

Another of Ferguson’s well-known sculptures is the “Figure-Eight Complement II” (see Figure 2.5 Color Plate IV, and Item 33 at the end of this chapter). It has been known for some time that the hyperbolic volume $V$ of the figure-eight knot complement is given by the formula

$$V = 2 \sqrt{3} \sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{k=n}^{2n-1} \frac{1}{k} \tag{2.11}$$

$$= 2.029883212819307250042405108549 \ldots \tag{2.12}$$

In 1998, British physicist David Broadhurst conjectured that $V/\sqrt{3}$ is a rational linear combination of $C_j = \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n (6n + j)^2}$.

Indeed, it is, as Broadhurst [60] found using a PSLQ program:

$$V = \frac{\sqrt{3}}{9} \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n} \left( \frac{18}{(6n + 1)^2} - \frac{18}{(6n + 2)^2} - \frac{24}{(6n + 3)^2} - \frac{6}{(6n + 4)^2} + \frac{2}{(6n + 5)^2} \right). \tag{2.14}$$

You can verify this yourself, using for example the Mathematician’s Toolkit, available at [http://www.experimentalmath.info]. Just type the following lines of code:

```mathematica
v = 2*sqrt[3] * sum[1/(n * binomial[2*n,n]) * sum[1/k, {k, n, 2*n-1}], {n, 1, infinity}]
pslq[v/sqrt[3], table[sum[(-1)^n/(27^n*(6*n+j)^2), {n, 0, infinity}], {j, 1, 6}]]
```
Figure 2.4. Ferguson’s “Eight-Fold Way” sculpture (see Color Plate IV). Courtesy of Helaman Ferguson.

Figure 2.5. Ferguson’s “Figure-Eight Knot Complement” sculpture (see Color Plate IV). Courtesy of Helaman Ferguson.
When this is done you will recover the solution vector \((9, -18, 18, 24, 6, -2, 0)\). A proof that formula (2.14) holds, together with a number of other identities for \(V\), is given at the end of this chapter in Items 34 and 35. As you will see, this proof is a classic example of a proof from experimental methodology, in that it relies on “knowing” ahead of time that the formula holds.

As we shall see in Section 3.4, constants given by a formula of the general type given in (2.14), namely a “BBP-type” formula, possess some remarkable properties, among them the fact that you can calculate the \(n\)-th digit (base-3 digit in this case) of such constants by means of a simple algorithm, without having to compute any of the first \(n - 1\) digits.

Ferguson comments that the discovery of this BBP-type expression for \(V\) is a “major advance toward understanding the figure-eight knot complement volume.” Accordingly, he has carved Broadhurst’s formula on the figure-eight knot complement sculptures commissioned by the Clay Mathematics Institute, both the Inner Mongolian black granite piece and the smaller bronzes (the Clay Math Award pieces). As he explains, “Finally the subtractive sculpture and the subtractive algorithm have come together.”

### 2.5 Recognition of Euler Sums

In April 1993, Enrico Au-Yeung, an undergraduate at the University of Waterloo, brought to the attention of one of us (Borwein) the curious result [42]

\[
\sum_{k=1}^{\infty} \left( 1 + \frac{1}{2} + \cdots + \frac{1}{k} \right)^2 k^{-2} = 4.59987\ldots \\
\approx \frac{17}{4} \zeta(4) = \frac{17\pi^4}{360}.
\]  

(2.15)

The function \(\zeta(s)\) in (2.15) is the classical \textit{Riemann zeta function},

\[
\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}.
\]

Bernoulli showed that for even integers, \(\zeta(2n)\) is a rational multiple of \(\pi^{2n}\) [49]. (Bernoulli’s result is proved in Section 3.2 of the second volume of this work)

Au-Yeung had computed the sum in (2.15) to 500,000 terms, giving an accuracy of 5 or 6 decimal digits. Suspecting that his discovery was
merely a numerical coincidence, Borwein sought to compute the sum to a higher level of precision. Using Fourier analysis and Parseval’s equation, he obtained

\[
\frac{1}{2\pi} \int_0^\pi (\pi - t)^2 \log^2 \left( \frac{t}{2} \right) \, dt = \sum_{n=1}^{\infty} \left( \sum_{k=1}^{n} \frac{1}{k^2} \right)^2 \frac{1}{(n+1)^2}.
\]  

(2.16)

The idea here is that the series on the right of (2.16) permits one to evaluate (2.15), while the integral on the left can be computed using the numerical quadrature facility of Mathematica or Maple. When he did this, he was surprised to find that the conjectured identity holds to more than 30 digits. We should add here that by good fortune, \( \frac{17}{360} = 0.047222\ldots \) has period one and thus can plausibly be recognized from its first six digits, so that Au-Yeung’s numerical discovery was not entirely far-fetched.

What Borwein did not know at the time was that Au-Yeung’s suspected identity follows directly from a related result proved by De Doelder in 1991 [85]. In fact, it had cropped up even earlier as a problem in the American Mathematical Monthly, but the story goes back further still. Some historical research showed that Euler considered these summations. In response to a letter from Goldbach, he examined sums that are equivalent to

\[
\sum_{k=1}^{\infty} \left( 1 + \frac{1}{2^m} + \cdots + \frac{1}{k^m} \right) (k+1)^{-n}.
\]  

(2.17)

The great Swiss mathematician was able to give explicit values for certain of these sums in terms of the Riemann zeta function. For example, he found an explicit formula for the case \( m = 1, \ n \geq 2 \).

In retrospect, perhaps it was for the better that Borwein had not known of De Doelder’s and Euler’s results, because Au-Yeung’s intriguing numerical discovery launched a fruitful line of research by a number of researchers that continued until nearly the present day. Sums of this general form are nowadays known as “Euler sums” or “Euler-Zagier sums.”

In order to explore them more rigorously, it has been necessary to develop an efficient means to calculate their value to high precision—namely the 200 or more digit accuracy needed to obtain numerically significant results using integer relation calculations. Along this line, one of us (Bailey [20]) found a satisfactory scheme involving the Euler-Maclaurin summation formula. Another, more powerful scheme is described in [44]. These techniques will be discussed in Section 7.5 of the second volume of this work.

High precision calculations of many of these sums, together with considerable investigations involving heavy use of Maple’s symbolic manipulation facilities, eventually yielded numerous new results.
Below are just a few of the interesting results that were first discovered numerically and have since been established analytically \cite{43}. Since these results were first obtained in 1994, many more specific identities have been discovered, and a growing body of general formulas and other results have been proven. These results, together with the underlying numerical and symbolic techniques used in their derivation, are discussed further in Chapter 3 of the second volume.

\[
\sum_{k=1}^{\infty} \left( 1 + \frac{1}{2} + \cdots + \frac{1}{k} \right)^2 (k+1)^{-4} = \frac{37}{22680} \pi^6 - \zeta^2(3),
\]

\[
\sum_{k=1}^{\infty} \left( 1 + \frac{1}{2} + \cdots + \frac{1}{k} \right)^3 (k+1)^{-6} = \zeta^3(3) + \frac{197}{24} \zeta(9) + \frac{1}{2} \pi^2 \zeta(7) - \frac{11}{120} \pi^4 \zeta(5) - \frac{37}{7560} \pi^6 \zeta(3),
\]

\[
\sum_{k=1}^{\infty} \left( 1 - \frac{1}{2} + \cdots + (-1)^{k+1} \frac{1}{k} \right)^2 (k+1)^{-3} = 4 \text{Li}_5 \left( \frac{1}{2} \right) - \frac{1}{30} \log^5(2) - \frac{17}{32} \zeta(5) - \frac{11}{720} \pi^4 \log(2) + \frac{7}{4} \zeta(3) \log^2(2) + \frac{1}{18} \pi^2 \log^3(2) - \frac{1}{8} \pi^2 \zeta(3),
\]

where \( \text{Li}_n(x) = \sum_{k>0} x^k/k^n \) denotes the polylogarithm function.

\subsection*{2.6 Quantum Field Theory}

In another recent development, David Broadhurst (who discovered the identity \eqref{2.14} for Ferguson’s Clay Math Award sculpture) has found, using similar methods, that there is an intimate connection between Euler sums and constants resulting from evaluation of Feynman diagrams in quantum field theory \cite{62, 63}. In particular, the renormalization procedure (which removes infinities from the perturbation expansion) involves multiple zeta values, which we will discuss in detail in Chapter 3 of the second volume.

Broadhurst’s recent results are even more remarkable. He has shown \cite{60}, using PSLQ computations, that in each of ten cases with unit or zero mass, the finite part of the scalar 3-loop tetrahedral vacuum Feynman diagram reduces to four-letter “words” that represent iterated integrals in an alphabet of seven “letters” comprising the single 1-form \( \Omega = dx/x \) and the six 1-forms \( \omega_k = dx/\left( \lambda^{-k} - x \right) \), where \( \lambda = (1+\sqrt{-3})/2 \) is the primitive
2.7. Definite Integrals and Infinite Series

Figure 2.6. The ten tetrahedral configurations.

sixth root of unity, and $k$ runs from 0 to 5. A four-letter word here is a four-dimensional iterated integral, such as

$$U = \zeta(\Omega^2 \omega_3 \omega_1) = \int_0^1 \frac{dx_1}{x_1} \int_0^{x_1} \frac{dx_2}{x_2} \int_0^{x_2} \frac{dx_3}{-1 - x_3} \int_0^{x_3} \frac{dx_4}{1 - x_4} = \sum_{j > k > 0} (-1)^j \cos(2\pi k/3) \frac{1}{j^3 k}.$$  

There are $7^4$ such four-letter words. Only two of these are primitive terms occurring in the 3-loop Feynman diagrams: $U$, above, and

$$V = \text{Re} \left[ \zeta(\Omega^2 \omega_3 \omega_1) \right] = \sum_{j > k > 0} (-1)^j \cos(2\pi k/3) \frac{1}{j^3 k}.$$  

The remaining terms in the diagrams reduce to products of constants found in Feynman diagrams with fewer loops. These ten cases are shown in Figure 2.6. In these diagrams, dots indicate particles with nonzero rest mass. The formulas that have been found, using PSLQ, for the corresponding constants are given in Table 2.1. In the table the constant $C = \sum_{k > 0} \sin(\pi k/3)/k^2$.

2.7. Definite Integrals and Infinite Series

We mention here one particularly useful application of experimental mathematics methodology: evaluating definite integrals and sums of infinite series by means of numerical calculations. In one sense, there is nothing new here, since mathematicians have utilized computers to compute the
approximate numerical value of definite integrals and infinite series since the dawn of computing. What we suggest here, however, is a slightly different approach: Use advanced numerical quadrature techniques and series summations methods, extended to the realm of high-precision arithmetic, and then use the computed values (typically accurate to tens or even hundreds of decimal digits) as input to a computer-based constant recognition tool, which hopefully can recognize the constant as a simple expression involving known mathematical constants.

We will discuss techniques for computing definite integrals and sums of series to high precision in Section 7.4 of the second volume of this work. For the time being, we simply note that both Mathematica and Maple have incorporated some reasonably good numerical facilities for this purpose, and it is often sufficient to rely on these packages when numerical values are needed.

For our first example, we use Maple or Mathematica to compute the

\begin{table}
\centering
\begin{tabular}{|l|}
\hline
$V_1$ &= $6\zeta(3) + 3\zeta(4)$ \\
$V_{2A}$ &= $6\zeta(3) - 5\zeta(4)$ \\
$V_{2N}$ &= $6\zeta(3) - \frac{13}{3}\zeta(4) - 8U$ \\
$V_{3T}$ &= $6\zeta(3) - 9\zeta(4)$ \\
$V_{3S}$ &= $6\zeta(3) - \frac{14}{3}\zeta(4) - 4C^2$ \\
$V_{3L}$ &= $6\zeta(3) - \frac{15}{3}\zeta(4) - 6C^2$ \\
$V_{4A}$ &= $6\zeta(3) - \frac{17}{3}\zeta(4) - 6C^2$ \\
$V_{4N}$ &= $6\zeta(3) - 14\zeta(4) - 16U$ \\
$V_5$ &= $6\zeta(3) - \frac{469}{6}\zeta(4) + \frac{7}{3}C^2 - 16V$ \\
$V_6$ &= $6\zeta(3) - 13\zeta(4) - 8U - 4C^2$ \\
\hline
\end{tabular}
\caption{Formulas found by PSLQ for the ten tetrahedral diagrams.}
\end{table}
following three integrals to over 100 decimal digit accuracy:

\[
\int_0^1 \frac{t^2 \log(t)}{(t^2 - 1)(t^4 + 1)} \, dt = 0.180671262590654942792308128981671615337114571018296766266
\]

\[
\int_0^{\pi/4} \frac{t^2}{\sin^2(t)} \, dt = 0.843511841685034634002620051999528151651689086421444293697
\]

\[
\int_0^{\pi} \frac{x \sin x}{1 + \cos^2 x} \, dx = 2.4674011002723396547086227499603778382842851810197656603
\]

The third of these is from [105]. Both Maple and Mathematica attempt to evaluate these definite integrals analytically. In each case, however, while the results appear to be technically correct, they are not very useful, in that they are either rather lengthy, or involve advanced functions and complex entities. We suspect that there are considerably simpler closed-form versions.

Indeed, using the Inverse Symbolic Calculator (ISC) tool (a constant recognition facility) at [http://www.cecm.sfu.ca/projects/ISC](http://www.cecm.sfu.ca/projects/ISC), we obtain the following, based solely on the numerical values above:

\[
\int_0^1 \frac{t^2 \log(t)}{(t^2 - 1)(t^4 + 1)} \, dt = \frac{\pi^2 (2 - \sqrt{2})}{32}
\]

\[
\int_0^{\pi/4} \frac{t^2}{\sin^2(t)} \, dt = -\frac{\pi^2}{16} + \frac{\pi \log(2)}{4} + G
\]

\[
\int_0^{\pi} \frac{x \sin x}{1 + \cos^2 x} \, dx = \frac{\pi^2}{4}, \tag{2.20}
\]

where \(G\) denotes Catalan’s constant

\[
G = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n + 1)^2}.
\]
We might add that Catalan’s constant is widely believed to be irrational, but this has never been proved. Using an integer relation tool, together with a high-precision numerical value of Catalan (which can easily be found by typing \texttt{N[Catalan, 100]} in Mathematica), you can see that it is not a root of an integer polynomial with reasonable degree and reasonable-sized coefficients.

As an exercise, we challenge you to evaluate
\[ \int_0^{\pi/4} \frac{t^3}{\sin^2(t)} \, dt. \]

Other examples of numerical identification of definite integrals will be presented in Section 7.4 of the second volume of this work.

As a second example, as we shall see in Section 3.1 rational linear combinations of arctangent formulas can be devised to produce relatively efficient algorithms for computing \( \pi \). In fact, such formulas have been used for centuries. One approach to finding such formulas is to analytically derive them. Another approach is to simply explore for them using the numerical values of individual arctan formulas. For instance, by computing values of the individual arctans below to moderately high precision, and applying an integer relation tool, one can easily deduce the relations
\[
\pi = 48 \arctan \frac{1}{49} + 128 \arctan \frac{1}{57} - 20 \arctan \frac{1}{239} + 48 \arctan \frac{1}{110443},
\]
\[
\pi = 176 \arctan \frac{1}{57} + 28 \arctan \frac{1}{239} - 48 \arctan \frac{1}{682} + 96 \arctan \frac{1}{12943}.
\]

One way to do this is by using the “Experimental Mathematician’s Toolkit,” which is available at \url{http://www.experimentalmath.info}. Type the string
\texttt{pslq[\pi, \arctan[1/49], \arctan[1/57], \arctan[1/239], \arctan[1/110443]]}
and you will obtain the vector \((1, -48, -128, 20, -48)\), which gives the first formula of (2.21). These particular formulas were used by Kanada in his latest computation of \( \pi \) to more than one trillion decimal digits.

A third example, one of the most remarkable examples of constant recognition in the literature, is due to Ronald Graham and Henry Pollak [100]. They were studying the sequences \((a_n)\) and \((b_n)\), defined by \(a_0 = m\), then
\[
a_{n+1} = \lfloor \sqrt{2a_n(a_n + 1)} \rfloor
\]
followed by
\[
b_n = a_{2n+1} - 2a_{2n-1}.
\]
Can the sequence \((a_n)\) and/or \((b_n)\) be identified? Graham and Pollak found that if you define the constants \(\alpha(m)\), for integers \(m \geq 1\),
\[
\alpha(m) = 0.b_1b_2b_3\cdots_2,
\]
meaning that the sequence \((b_n)\) is to be interpreted as the binary expansion of the constant \(\alpha(m)\), then the resulting constants are simple algebraic numbers. In particular,
\[
\begin{align*}
\alpha(1) &= \sqrt{2} - 1 \\
\alpha(2) &= \sqrt{2} - 1 \\
\alpha(3) &= 2\sqrt{2} - 2 \\
\alpha(4) &= 2\sqrt{2} - 2 \\
\alpha(5) &= 3\sqrt{2} - 4 \\
\alpha(6) &= 4\sqrt{2} - 5 \\
\alpha(7) &= 3\sqrt{2} - 4 \\
\alpha(8) &= 5\sqrt{2} - 7 \\
\alpha(9) &= 4\sqrt{2} - 5 \\
\alpha(10) &= 6\sqrt{2} - 8.
\end{align*}
\]
This recognition led to an explicit formula for the sequence \((a_n)\) as
\[
a_n = \lfloor \tau(2^{(n-1)/2} + 2^{(n-1)/2}) \rfloor, \tag{2.25}
\]
where \(\tau\) is the \(m\)-th smallest real number in the set \(\{1, 2, 3, \cdots\} \cup \{\sqrt{2}, 2\sqrt{2}, 3\sqrt{2}, \cdots\}\). See [100] for complete details. It is not known if generalized sequences such as
\[
\begin{align*}
a_{n+1} &= \lfloor \sqrt{3}a_n(a_n + 1) \rfloor \tag{2.26} \\
a_{n+1} &= \lfloor \sqrt{2}a_n(a_n + 1)(a_n + 2) \rfloor \tag{2.27}
\end{align*}
\]
have analogous properties.

We will discuss constant recognition techniques more in Section 6.3.

2.8 Prime Numbers and the Zeta Function

The oldest systematic treatment of prime numbers is in Euclid’s *Elements*, written about 300 BCE. Euclid’s results on prime numbers, like his results on geometry, are presented entirely as theorems and proofs, with scarcely
any motivating examples or mention of how these results were first discovered. Thus it is not possible to learn to what extent experimental methods were used in the original discovery of these principles. In more recent times, we have written accounts of the discoveries of various prime number results, and we can find several clear examples of experimental mathematics in action. As a canonical example, in 1849 Gauss recounted his analysis of the density of prime numbers:

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 \( \int_2^x dt/\log t \). [102, 98]

Formal proof that the above approximation is asymptotically correct, which is now known as the Prime Number Theorem, did not come until 1896, more than 100 years after Gauss’ experimental discovery [77]. In his writings on the subject, Gauss expressed a fascination with prime numbers that is reminiscent of the fascination other mathematicians have expressed with the digits of \( \pi \):

The problem of distinguishing prime numbers from composite numbers and of resolving the latter into their prime factors is known to be one of the most important and useful in arithmetic. It has engaged the industry and wisdom of ancient and modern geometers to such an extent that it would be superfluous to discuss the problem at length. . . . Further, the dignity of the science itself seems to require that every possible means be explored for the solution of a problem so elegant and so celebrated. [95, Article 329 (1801)]

This fascination with prime numbers has not diminished in the 201 years since this was written. Compare for example the comments of Don Zagier, in a recent article analyzing the first 50 million prime numbers:

[T]here is no apparent reason why one number is prime and another not. To the contrary, upon looking at these numbers one has the feeling of being in the presence of one of the inexplicable secrets of creation. [195]

In recent years, with the advent of computers, the prime-counting function \( \pi(x) \) has been tabulated precisely for rather large values of \( x \). This has been done by using some rather advanced techniques that we will not describe here. Interested readers are referred to the new book, Prime Numbers: A Computational Perspective, by Richard Crandall and Carl Pomerance [77], where two different advanced techniques are presented. Table 2.2 gives values of \( \pi(x) \) for powers of ten up to \( 10^{22} \), together with the
corresponding values of the approximate formula given by the Prime Number Theorem, and the differences \( \int_2^x dt/\log t - \pi(x) \). The last-listed and most recent calculation is due to P. Demichel and X. Gourdon (February 2001). This data was obtained from Eric Weisstein’s very useful “World of Mathematics” web site [http://mathworld.wolfram.com].

One of the principal motivations of computing values of the prime-counting function \( \pi(x) \) is to explore a fascinating and highly promising connection to the Riemann zeta function, a discovery which is a classic example of an experimental approach to mathematical research. The following material is adapted in part from an excellent and very readable article by Andrew Granville [102].

In examining the data in Table 2.2, we observe that the overcount values in the last column appear to be roughly \( \sqrt{x} \). Thus one might think that

<table>
<thead>
<tr>
<th>( x )</th>
<th>( \pi(x) )</th>
<th>( \int_2^x dt/\log t )</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>10^1</td>
<td>4</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>10^2</td>
<td>25</td>
<td>29</td>
<td>4</td>
</tr>
<tr>
<td>10^3</td>
<td>168</td>
<td>177</td>
<td>9</td>
</tr>
<tr>
<td>10^4</td>
<td>1229</td>
<td>1245</td>
<td>16</td>
</tr>
<tr>
<td>10^5</td>
<td>9592</td>
<td>9629</td>
<td>37</td>
</tr>
<tr>
<td>10^6</td>
<td>78498</td>
<td>78627</td>
<td>129</td>
</tr>
<tr>
<td>10^7</td>
<td>6 64579</td>
<td>6 64917</td>
<td>338</td>
</tr>
<tr>
<td>10^8</td>
<td>57 61455</td>
<td>57 62208</td>
<td>753</td>
</tr>
<tr>
<td>10^9</td>
<td>508 47534</td>
<td>508 49234</td>
<td>1700</td>
</tr>
<tr>
<td>10^{10}</td>
<td>4550 52511</td>
<td>4550 55614</td>
<td>3103</td>
</tr>
<tr>
<td>10^{11}</td>
<td>41180 54813</td>
<td>41180 66400</td>
<td>11587</td>
</tr>
<tr>
<td>10^{12}</td>
<td>3 76079 12018</td>
<td>3 76079 50280</td>
<td>38262</td>
</tr>
<tr>
<td>10^{13}</td>
<td>34 60655 36839</td>
<td>34 60656 45809</td>
<td>1 08970</td>
</tr>
<tr>
<td>10^{14}</td>
<td>320 49417 50802</td>
<td>320 49420 65691</td>
<td>3 14889</td>
</tr>
<tr>
<td>10^{15}</td>
<td>2984 45704 22669</td>
<td>2984 45714 75287</td>
<td>10 52618</td>
</tr>
<tr>
<td>10^{16}</td>
<td>27923 83410 33925</td>
<td>27923 83442 48556</td>
<td>32 14631</td>
</tr>
<tr>
<td>10^{17}</td>
<td>2 62355 71576 54233</td>
<td>2 62355 71656 10821</td>
<td>79 56588</td>
</tr>
<tr>
<td>10^{18}</td>
<td>24 73995 42877 40860</td>
<td>24 73995 43096 90414</td>
<td>219 49554</td>
</tr>
<tr>
<td>10^{19}</td>
<td>234 05766 72763 44607</td>
<td>234 05766 73762 22381</td>
<td>998 77774</td>
</tr>
<tr>
<td>10^{20}</td>
<td>2220 81960 25609 18840</td>
<td>2220 81960 27836 63483</td>
<td>2227 44643</td>
</tr>
<tr>
<td>10^{21}</td>
<td>21127 26948 60187 31928</td>
<td>21127 26948 66161 26181</td>
<td>5973 94253</td>
</tr>
<tr>
<td>10^{22}</td>
<td>2 01467 28668 93159 06290</td>
<td>2 01467 28669 12482 61497</td>
<td>19323 55207</td>
</tr>
</tbody>
</table>

Table 2.2. The prime-counting function \( \pi(x) \) and Gauss’ approximation.
Figure 2.7. Page 1 of Riemann’s 1859 manuscript. Courtesy of Niederschlesische Staats- und Universitätsbibliothek Göttingen.
2.8. Prime Numbers and the Zeta Function

Figure 2.8. Page 2 of Riemann's 1859 manuscript. Courtesy of Niederschlesische Staats- und Universitätsbibliothek Göttingen.
by subtracting \( \sqrt{x} \), one would get an asymptotically better approximation. This is not the case—in 1914, Littlewood proved that the differences between \( \pi(x) \) and Gauss’ approximation change sign infinitely often. In 1933, Skewes showed that the first sign change must occur at least by \( 10^{10^{10^3}} \), a number known as the Skewes number because of its prodigious size (see [77], Exercise 1.35). This bound has recently been reduced to a “tiny” number, a mere \( 10^{316} \) [102]. Littlewood [143, pg. 110–112] gives a fascinating discussion of his interaction with Skewes.

A key development in this area stems from Riemann’s discovery in 1859 that

\[
\frac{\pi(x) - \int_2^x \frac{dt}{\log t}}{\sqrt{x}/\log x} \approx -1 - 2 \sum_{\gamma \in S} \frac{\sin(\gamma \log x)}{\gamma},
\]

where \( S \) is the set of \( \gamma \) such that \( \gamma > 0 \) and \( 1/2 + i\gamma \) is a zero of the Riemann zeta function \( \zeta(s) = \sum_{k>0} 1/k^s \). The left-hand side of (2.28) is simply the overcount noted in Table 2.2, divided by what we earlier observed to be the apparent size of the error term, namely \( \sqrt{x}/\log x \) (a more accurate version of the approximation \( \sqrt{x} \)). The right-hand side of (2.28) is suggestive of a Fourier series—it is as if the prime numbers have “music” in them.

In Riemann’s 1859 memoir, in which he presented this approximation formula (2.28), he noted that the result was contingent upon (actually equivalent to) the hypothesis that the only zeroes of \( \zeta(s) \) for complex numbers \( s = \sigma + i\gamma \) with \( 0 \leq \sigma \leq 1 \) are for \( \sigma = 1/2 \) [172]. This is the famous Riemann Hypothesis, whose proof has eluded the best mathematicians for nearly 150 years. Photocopies of the first two pages of Riemann’s memoir on the zeta function, stored in Göttingen, are shown in Figures 2.7 and 2.8.

Riemann’s 1859 memoir did not contain any clues as to how he was led to make this conjecture. For many years mathematicians believed that Riemann had come to this conjecture on the basis of some profound intuition. Indeed, the Riemann Hypothesis has been held up as a premier example of the heights one could attain by sheer intellect alone. In 1929, long after Riemann’s death, the renowned number theorist Carl Ludwig Siegel (1896–1981) learned that Riemann’s widow had donated his working papers to the Göttingen University library. Among these papers Siegel found several pages of heavy-duty numerical calculations, with a number of the lowest-order zeroes of the zeta function calculated to several decimal places each. As Andrew Granville has observed, “So much for pure thought alone” [102]. The Riemann-Siegel formula is developed further in Item 2 of Chapter 3 in the second volume.

In 1936 Cramer proposed a probabilistic model of the primes. In particular, he defined a sequence \( X_3, X_4, \ldots \) of independent random variables
on \(\{0,1\}\) with \(P(X_n = 1) = 1/\log n\), and \(P(X_n = 0) = 1 - 1/\log n\) (here, \(P\) denotes probability). This turns out to be a fairly good model for occurrence of prime numbers. In fact, it can be shown that

\[
\lim_{n \to \infty} \frac{\sum_{x \leq n \leq x+h} X_n}{\int_x^{x+h} dt / \log t} = 1
\]  
(2.29)

with probability 1. In such comparisons of statistical distributions, it is natural to consider the variance,

\[
V = E \left( \sum_{x \leq n \leq x+h} X_n - \int_x^{x+h} \frac{dt}{\log t} \right)^2.
\]  
(2.30)

(here, \(E\) denotes expected value). Unfortunately, it can be shown that this variance is not the same as the corresponding statistical variance of the prime counting function \(\pi(x)\). In Figure 2.9, we show 100 zeroes of the zeta function, beginning with the \((10^{21} + 1)\)-th zero, displayed as the dotted line, with pseudo-random numbers (added and scaled to the endpoints of the graph) displayed as the dashed line for comparison. The ranks of the zeroes, minus \((10^{21} + 1)\), are plotted on the \(x\)-axis, while the imaginary parts of the zeroes, minus the imaginary part of the \((10^{21} + 1)\)-th zero (namely 144176897509546973538.498...), are plotted on the \(y\) axis. It is clear from this plot that the zeroes of the Riemann zeta function are hardly “randomly” spaced—they adhere to a straight line much more closely than the pseudorandom data. It is as if the zeroes of the Riemann zeta function consciously “repel” each other, so as to stay much closer to constant spacing.

Given how well Gauss’ model has worked in the past, this breakdown was both unexpected and disconcerting. As Paul Erdős wrote, “God may not play dice with the universe, but something strange is going on with the primes.” [147]

In 1976, Julia Mueller revisited the question of the variance of the prime counts in her PhD dissertation. Building on her work, Daniel Goldston and Hugh Montgomery soon made the remarkable discovery that a good understanding of the variance is actually equivalent to the spacing between pairs of zeroes of the zeta function. Three years earlier, while investigating a different question of number theory, Montgomery had been led to the following conjecture: The expected number of zeroes of the zeta function in a gap of length \(T\) times the average gap, following a zero, is

\[
\int_0^T \left( 1 - \left( \frac{\sin \pi u}{\pi u} \right)^2 \right) du.
\]  
(2.31)
If the zeroes of the zeta function were randomly spaced, this value would simply be \( T \). This conjecture agrees with the observed repulsion of zeroes, as observed in Figure 2.9. For example, we would expect to find another zero within 0.01 times the average spacing roughly one time in 100 trials for random spacing, whereas this formula predicts that such close spacing would occur only one time in nearly 1,000,000 instances. We can compare how closely this data matches with actual nearest-neighbor spacing for the zeta function, by examining calculated data by Andrew Odlyzko [159]. Figure 2.10 shows this spacing data based on a billion zeroes near the \( 1.3 \times 10^{16} \)-th zero.

As you can see from this graph, this function agrees extremely well with the experimentally measured spacings. Montgomery has now partially proven that his conjecture is correct—he has shown that the Fourier transform of his distribution function is correct in a small range, assuming the Riemann Hypothesis.
The next step in this saga is even more remarkable. Soon after his experimental discovery on the prime counts and zero spacing, Montgomery visited the Institute for Advanced Study in Princeton, hoping to discuss his new ideas with Selberg and Bombieri, who were both at the Institute at the time. In a communal afternoon tea, Montgomery happened to chat with Freeman Dyson, the renowned mathematical physicist (although he originally was a number theorist). When Montgomery told Dyson of his new ideas on the zeroes of the Riemann zeta function, Dyson responded that he was very familiar with this problem, and in fact was even aware of the issue of the spacing of the zeroes. But it wasn’t from number theory that Dyson was aware of these phenomena; instead, Dyson had encountered these questions through quantum mechanics. In fact, Montgomery’s
distribution was precisely the function that Dyson had found ten years earlier when modeling energy levels in quantum chaos. These researchers immediately realized that this serendipitous coincidence would likely lead to more progress on both the number theory and quantum physics fronts.

The quantum chaos equations are comparatively simpler than those of prime number theory, and so they were better understood. As a result, there was a flurry of new activity in the field. Researchers focused not only on close pairs of zeroes, but also three-at-a-time correlations and $n$-at-a-time correlations. However, it was 20 years later (1994) before Rudnick and Sarnak proved the quantum mechanics analogue of Montgomery’s result (that the Fourier transform of the distribution function is correct in a small range, assuming the Riemann Hypothesis) [175]. Then in 1996, two mathematical physicists (Bogolmony and Keating) rederived the Montgomery-Dyson prediction for $n$-at-a-time correlations from a new angle. They took a classic conjecture of number theory, namely the Hardy-Littlewood version of the prime $k$-tuplets conjecture, and showed that this also led to a similar conclusion [39]. Since then there has been a flurry of new research in this area, both on the number theory and mathematical physics fronts. These developments have led some in the field to optimistically predict that the long-sought proof of the Riemann Hypothesis may be at hand. As Michael Berry said in 2000,

I have a feeling that the Riemann Hypothesis will be cracked in the next few years. I see the strands coming together. Someone will soon get the million dollars. [129]

The million dollars Berry mentions here refers to a prize that has been offered for the proof of the Riemann Hypothesis (and for several other outstanding mathematical problems) by the Clay Mathematics Institute. Details of this prize are available on the Clay Institute web site [http://www. claymath.org](http://www.claymath.org). A very readable recent survey is to be found in [72].

### 2.9 Two Observations about $\sqrt{2}$

As we observed earlier in the discussion of Pascal’s triangle, it is still possible to find new insights even in the oldest areas of mathematics. We illustrate this principle again with two intriguing observations on that oldest of irrational constants, the square root of two.
2.9. Two Observations about $\sqrt{2}$

2.9.1 Irrationality

We first present Tom Apostol’s lovely new geometric proof of the irrationality of $\sqrt{2}$ [6].

**Proof.** To say $\sqrt{2}$ is rational is to draw a right-angled isosceles triangle with integer sides. Consider the smallest right-angled isosceles triangle with integer sides—that is with shortest hypotenuse.

Suppose ABC is that triangle with apex A and hypotenuse AC. Draw a circle centered at A of length AB and mark the point D where it cuts the hypotenuse. Now draw the tangent to the circle at D and mark the point E where it cuts the base of the triangle. Then DEC is a smaller isosceles right-angled triangle and again has integer sides (see Figure 2.11 and Color Plate II). This is a contradiction.

As Figure 2.11 suggests, this can be beautifully illustrated in a dynamic geometry package such as Geometer’s Sketchpad or Cinderella. We can continue to draw smaller and smaller integer-sided similar triangles until the area drops below $\frac{1}{2}$. But we give it here to emphasize the ineffably human component of the best proofs, and to suggest the role of the visual.

Algebraically this leads to the following proof that nonperfect squares...
have irrational roots: If \( \frac{p}{q} = \sqrt{n} \), then
\[
\frac{p'}{q'} = \frac{nq - \lfloor \sqrt{n} \rfloor p}{p - \lfloor \sqrt{n} \rfloor q} = \frac{p}{q}
\] (2.32)
and \( 0 < p' < p, 0 < q' < q \). It is left to the reader to convert this into a picture along the lines of Figure 2.11.

### 2.9.2 Rationality

Ironically, \( \sqrt{2} \) can sometimes make things rational:
\[
\left( \sqrt{2} \right)^2 = 2
\] (2.33)

Hence, by the principle of the excluded middle,

\[
\text{either } \sqrt{2} \in \mathbb{Q} \text{ or } \sqrt{2} \notin \mathbb{Q}.
\]

In either case, we can deduce that there are irrational numbers \( \alpha \) and \( \beta \) with \( \alpha^\beta \) rational. But how do we know which ones? This is not an adequate proof for an Intuitionist nor a Constructivist. It is entirely ineffective, and we may build a whole mathematical philosophy project around such issues. Actually, \( \sqrt{2}^\sqrt{2} \) is transcendental by the Gelfond-Schneider theorem (Exercise 28), but proofs of this are hard and usually suffer from the same flaws.

It is instructive to compare this result with the assertion that \( \alpha = \sqrt{2} \) and \( \beta = 2 \log_2(3) \) yield \( \alpha^\beta = 3 \) as Mathematica confirms. This illustrates nicely that verification is often easier than discovery. Similarly, the fact that multiplication is easier than factorization is at the base of secure encryption schemes for e-commerce.

Indeed, there are eight possible rational/irrational triples: \( \alpha^\beta = \gamma \); finding examples of all cases is now a good exercise (Exercise 29). Note how much can be taught about computation with rational numbers, approximation to irrationals, rates of convergence, etc. from these simple pieces.

We close the section with a description of the meeting between the inventor of logarithms (John Napier) and the scientist who made them into technology (Henry Briggs)

[W]here almost one quarter hour was spent, each beholding the other with admiration before one word was spoken: at last Mr. Briggs began “My Lord, I have undertaken this long journey purposely to see your person, and to know by what wit or ingenuity you first
came to think of this most excellent help unto Astronomy, viz. the Logarithms: but my Lord, being by you found out, I wonder nobody else found it out before, when now being known it appears so easy.”

2.10 Commentary and Additional Examples

1. **The hardest possible proof?** Use Fermat’s last theorem to prove $2^{1/n}$ is irrational for integer $n > 2$. Generalize.

2. **The final digit of a sum.** Problem: Determine the final digit $\ell_n$ of $\sigma_n = \sum_{k=1}^{n} k$. (Taken from [105]).

   Solution: Computational experimentation shows the pattern repeats modulo 20; $\ell_{n+20} = \ell_n \mod 20$ is easily proven from $\sigma_{n+20} = \sigma_n + \sum_{n+1}^{n+20} k$.

3. **The 3x+1 problem.** This is a classic example of an innocent looking, but highly intractable problem:

   For integer $x$, let $T(x) = (3x + 1)/2$ for $x$ odd and $x/2$ for $x$ even. The 3x + 1 conjecture is that starting from any positive integer $n$, repeated iteration of $T$ eventually returns to 1.

   This problem is best described in the interactive article by Jeff Lagarias at [http://www.cecm.sfu.ca/organics/papers/lagarias](http://www.cecm.sfu.ca/organics/papers/lagarias) (see also [137]), with records stored at [http://www.ieeta.pt/~tos/3x+1.html](http://www.ieeta.pt/~tos/3x+1.html). This conjecture has been “checked” to at least $100 \cdot 2^{50}$.

4. **Limit of a simple iteration.** Establish the limit of the iteration that starts with $a_0 = 0, a_1 = 1/2$ and iterates $a_{n+1} = (1 + a_n + a_{n-1}^3)/3$, for $n > 1$. Determine what happens as $a_1 = a$ is allowed to vary.

5. **Putnam problem 1985–B5.** Evaluate

   $$ K = \int_0^\infty t^{-1/2} e^{-1985(t+t^{-1})} \, dt. $$

   Answer: $K = \sqrt{\pi} e^{-3970/\sqrt{1985}}$. The Putnam problems listed here and in subsequent chapters are taken from [127]. *Hint:* This is problematic to evaluate numerically as stated, since its value is tiny. So consider instead $K(\alpha) = \int_0^\infty t^{-1/2} e^{-\alpha(t+t^{-1})} \, dt$ for some other specific (or general) constant $\alpha$. 

6. **Putnam problem 1987–A6.** Let $n$ be a positive integer and let $a_3(n)$ be the number of zeroes in the ternary expansion of $n$. Determine for which positive $x$ the series $\sum_{n=1}^{\infty} x^{a_3(n)}/n^3$ converges. Answer: For $x < 25$. In the $b$-ary analogue, $\sum_{n=1}^{\infty} x^{a_b(n)}/n^b$ converges if and only if $x < b^b - b + 1$.

7. **Putnam problem 1987–B1.** Evaluate

$$\int_2^4 \frac{\sqrt{\log (9 - x)}}{\sqrt{\log (9 - x) + \sqrt{\log (3 + x)}}} \, dx \quad (= 1).$$

8. **Putnam problem 1991–A5.** Find the supremum of

$$\int_0^y \sqrt{x^4 + (y - y^2)^2} \, dx,$$

for $0 \leq y \leq 1$. *Hint:* Plot the function.

9. **Putnam problem 1992–A2.** Evaluate

$$\int_0^1 C(-y - 1) \sum_{k=1}^{1992} \frac{1}{y + k} \, dy,$$

where $C(\alpha)$ is the coefficient of $x^{1992}$ in the Maclaurin expansion of $(1 + x)^{\alpha}$. Answer: 1992.

10. **Putnam problem 1992–B3.** Consider the dynamical system generated by $a_0 = x$ and

$$a_{n+1} = \frac{y^2 + a_n^2}{2},$$

for $n \geq 0$. Determine the region in the plane for which the iteration converges. What is its area? *Hint:* Try computing some values and plot the results. Assuming without loss of generality $x, y > 0$, the limit must satisfy $2\ell - \ell^2 = y^2$. Thus the region defined is the convex hull of unit circles centered at $(\pm 1, 0)$. Answer: $\pi + 4$.

11. **Random projections.** Consider an arbitrary point inside a triangle. Determine what happens asymptotically when the point is projected to successive sides of the triangle, where the side is selected either in cyclical order or pseudo-randomly. *Hint:* Consider first what happens in an obtuse triangle.
2.10. Commentary and Additional Examples

12. **Putnam problem 1995–B4.** Determine a simple expression for

\[
\sigma = \sqrt[8]{2207 - \frac{1}{2207 - \frac{1}{\ldots}}}. \quad (2.34)
\]

*Hint:* Calculate this limit to 15 decimal place accuracy, using ordinary double-precision arithmetic. Then use the ISC tool, with the “integer relation algorithm” option, to recognize the constant as a simple algebraic number. The result can be proved by noting that \(\sigma^8 = 2207 - 1/\sigma^8\), so that \(\sigma^4 + 1/\sigma^4 = 47\). Answer: \((3 + \sqrt{5})/2\).

13. **Berkeley problem 1.1.35.** Find the derivative at \(x = 0\) of

\[
\int_{\cos(x)\sin(x)}^{\cos(x)\sin(x)} e^{t^2+xt} dt.
\]

*Hint:* Plot it. Answer = \((e-3)/2\). The Berkeley problems listed here and in subsequent chapters are taken from [83].

14. **Berkeley problem 7.6.6.** Compute \(A^{10^6}\) and \(A^{-7}\) for

\[
A = \begin{bmatrix}
3/2 & 1/2 \\
-1/2 & 1/2
\end{bmatrix}.
\]

*Hint:* Use Mathematica or Maple to evaluate \(A^n\) for various integers \(n\).

15. **Two radical expressions.** (From [112] pg. 81, 84). Express

\[
\sqrt[3]{ \cos \left( \frac{2}{7} \pi \right) } + \sqrt[3]{ \cos \left( \frac{4}{7} \pi \right) } + \sqrt[3]{ \cos \left( \frac{6}{7} \pi \right) }
\]

\[
\sqrt[3]{ \cos \left( \frac{2}{9} \pi \right) } + \sqrt[3]{ \cos \left( \frac{4}{9} \pi \right) } + \sqrt[3]{ \cos \left( \frac{8}{9} \pi \right) }
\]

as radicals. *Hint:* Calculate to high precision, then use the ISC tool to find the polynomial they satisfy.

Answers: \(\sqrt[3]{\frac{1}{2}(5 - 3\sqrt{7})}\) and \(\sqrt[3]{\frac{3}{2} \sqrt{9} - 3}\).

16. **Some simple continued fractions.** Compute the simple continued fraction for \(e, (e - 1)/2, e^2, \log(2), \log(10), 3^{1/2}, 2^{1/3}, \pi, \pi/2, e^\pi, \) and \(\pi^e\).
17. **Crandall’s continued fraction.** Compute, then guess and prove, the continued fraction for

\[ \frac{e^{\sqrt{2}} + 1}{e^{\sqrt{2}} - 1}, \]

which fraction is manifestly not periodic, proving in this way that \( e^{\sqrt{2}} \) is irrational. Richard Crandall informs us that this (in 1968) was the first and perhaps only interesting thing he ever proved all by himself.

18. **Putnam problem 1988–B2.** Prove or disprove: If \( x \) and \( y \) are real numbers with \( y \geq 0 \) and \( y(y + 1) \leq (x + 1)^2 \), then \( y(y - 1) \leq x^2 \). *Hint:* Plot it.

19. **Putnam problem 1989–A3.** Show that all roots of

\[ 11z^{10} + 10iz^9 + 10iz - 11 = 0 \]

lie on the unit circle. *Hint:* This can be solved explicitly using Maple, Mathematica, or a custom-written root-finding program that employs Newton iterations. A detailed discussion of polynomial root-finding techniques can be found in Section 7.3 of the second volume.

20. **Putnam problem 1992–A3.** For a given positive integer \( m \) find all triples \((n, x, y)\) of positive integers with \((n, m) = 1\) solving \((x^2 + y^2)^n = (xy)^n\). *Hint:* Using a symbolic math program, try finding solutions for various integer pairs \( x, y \). Answer: The only solution is \((m + 1, 2^{m/2}, 2^{m/2})\) for \( m \) even.

21. **Berkeley problem 6.11.5.** Prove that \( \sqrt{2} + \sqrt{3} \) is irrational. *Hint:* Use Maple or Mathematica to find the minimum polynomial of this constant.

22. **Fateman’s web integrator.** Richard Fateman maintains an online integration tool, [http://torte.cs.berkeley.edu:8010/tilu](http://torte.cs.berkeley.edu:8010/tilu). In its early days, as many as two of every three requests were ill-formed; to address this, the interface performs a significant amount of heuristic work to decide what users intend by expressions such as

\[ \int \frac{ax + bx}{cx + dx} \, dx \quad \text{or} \quad \int \sin x \, dx. \]

The tool also runs directly on the Macintosh graphing calculator.
23. **The happy end problem.** The happy end problem is to find, for \( n \geq 3 \), the smallest positive integer \( N(n) \) such that any set of \( N(n) \) points, no three of which are collinear, must contain \( n \) points that are the vertices of a convex \( n \)-gon. It is so called because Ester Klein, who posed the problem, married George Szekeres shortly after he and Paul Erdős proved the first bounds on the problem \cite{144}. It is still open \cite{144}.

24. **The Mann iteration.** For any continuous function \( f : [0, 1] \mapsto [0, 1] \), the iteration \( x_0 = x \in [0, 1] \) and

\[
x_n = \frac{1}{n} \sum_{k=0}^{n-1} f(x_k)
\]

(the Cesaro average) always converges to a fixed point of \( f \). One can study many other summability methods similarly. Since the function can be highly obstreperous, this is largely a theoretical real-variable iteration, albeit a beautiful one. Easy examples will convince one of how painfully slow or unstable convergence can be. This is especially understandable in light of

**Theorem 2.1. (Sharkovsky).** If a continuous self-mapping of the reals, \( f \), possesses a periodic point of order \( m \), then \( f \) will possess a periodic point of order \( n \), precisely when \( n \) follows \( m \) in the following ordering of the natural numbers:

\[
3 > 5 > 7 > \cdots > 2^3 > 2^5 > 2^7 > \cdots > 2^n > 2^{n-1} > \cdots > 2 > 1.
\]

In particular this includes the famous result of Li and Yorke to the effect that “period three implies chaos.”

25. **Finding coefficients of an integer polynomial.** The numerical identification methods described here work especially well when you know a priori that a given integral, sum or other constant is a linear combination of given quantities, and you wish only to obtain the precise integer coefficients. For example, if you are told that, for any integer \( N > 0 \),

\[
\sum_{n=0}^{\infty} \frac{n^n e^{-n}}{(n+N)!}
\]
evaluates to a polynomial of degree $N$ in $e$, then it is an easy matter, for any given small $N$, to pick off the integers. Indeed, for $N < 10$, say, you can discover that
\[
Q_N = \sum_{n=0}^{\infty} \frac{n^n e^{-n}}{(n+N)!} - \sum_{k=1}^{N} \frac{(-1)^{k-1} e^k}{(N-k)! k^k}
\] (2.35)
is a rational number. The first four are $-1, -1/4, -7/108, -97/6912$.
Continuing in this manner, you can ultimately discover that
\[
Q_N = \sum_{k=1}^{N} \frac{(-1)^k}{(N-k)! k^k} \sum_{n=0}^{k-1} \frac{k^n}{n!}.
\] (2.36)
This relies on replacing $\exp(-n)$ by its series, exchanging order of summation, and then discovering and deriving the identity
\[
\sum_{k=0}^{n} (-1)^k k^n \binom{N+n}{N+k} = (-1)^n \sum_{k=1}^{N} k^n (-1)^{k-1} \binom{N+n}{N-k}
\] (2.37)
or equivalently,
\[
\sum_{k=0}^{M+N} (-1)^k (M-k)^M \binom{M+N}{k} = 0
\] (2.38)
for all $M, N > 0$. This in turn follows (using the binomial theorem) from
\[
\sum_{k=0}^{P} (-1)^k \binom{P}{k} = 0,
\] (2.39)
for all $0 \leq n < P$. The final identity (2.39) is established by setting $D^k f(x) = x^f^{(k)}(x)$ and observing that $D^k (1 - x)^P$ has a zero at $1$ for $k < P$.

26. A taste of J. E. Littlewood’s Miscellany. We record a variety of observations, mathematical, stylistic and personal from Littlewood’s wonderful Miscellany, a collection originally published in 1953, but republished with an excellent introduction by Béla Bollobás in 1988 [143]. More of Littlewood is to be found at the end of Chapter 4 of the second volume.
Figure 2.12. Duijvestijn’s dissection. Courtesy of Bela Bollobas.

(a) (Entry (10) page 28) Dissection of squares and cubes into squares and cubes, finite in number and all unequal. “The square dissection is possible in an infinity of different ways (the simplest, due to Duijvestijn, is shown in Figure 2.12). A cube dissection is not possible.” The proof of the second is short and elegant.

(b) (Entry (19) page 32) An isoperimirical problem: an area of (greatest) diameter not greater than 1 is at most $\frac{1}{4}\pi$.

Outline: “It is easy to see that we may suppose the area convex
and on one side of one of its ‘tangents’.” With polar coordinates

\[ \text{area} = \frac{1}{2} \int_{0}^{\frac{\pi}{2}} \left( r^2(\theta) + r^2(\theta - \frac{\pi}{2}) \right) d\theta, \]

and the integrand never exceeds one.

(c) (Page 38) Kakeya’s problem. “Find the region of least area in which a segment of unit length can turn continuously through 360° (minimize the area swept over). It was long thought that the answer was as in Figure 2.13 and the area \( \frac{1}{8} \pi \). In 1930 [sic], however, A. S. Besicovitch, (Math. Zeit. 27 (1928), 312–320.) showed that the answer is zero area (unattained): given an arbitrarily small \( \epsilon \) the area swept can be less than \( \epsilon \).”

(d) (§2, Misprints, page 56)

“I once challenged Hardy to find a misprint on a certain page of a joint paper. He failed: it was in his own name ‘G, H. Hardy’.”

“A minute I wrote (about 1917) for the Ballistics office ended with the sentence ‘Thus \( \sigma \) should be made as small as possible.’ This did not appear in the printed minute. But P. J. Brigg said ‘What is that?’ A speck in the blank space turned out to be the tiniest \( \sigma \) I have ever seen (the printers must have scoured London for it.).”

27. The hypocycloid. Cartesian coordinates are given by

\[ x = (a - b) \cos(t) + b \cos \left( \frac{(a/b - 1)t}{b} \right), \]
\[ y = (a - b) \sin(t) - b \sin \left( \frac{(a/b - 1)t}{b} \right) \]

for \( a > b > 0 \). This is plotted for \( a = 1, b = 2/3 \) in Figure 2.13.

An excellent source for curves is http://www-gap.dcs.st-and.ac.uk/~history/Curves/Curves.html

28. The Gelfond-Schneider theorem. This is the result that for complex algebraic numbers \( \alpha \neq 0, 1 \) and \( \beta \) irrational, the quantity \( \alpha^\beta \) is transcendental. It follows that

(a) \( \sqrt[3]{2} \) is transcendental; and

(b) \( e^\pi = (-1)^{-i} \) is transcendental.

29. Eight solutions. Find examples of all eight rational and irrational possibilities of \( \alpha^\beta = \gamma \).
2.10. Commentary and Additional Examples

30. Quantum connections. Another connection between quantum theory and the Riemann zeta is the observation, by Richard Crandall in 1991, that there exists an initial wave function $\psi(x, 0)$—having no zero-crossings whatever (it looks like a “bell curve,” for example)—which, under standard Schroedinger propagation, has evolved at a certain time $T$ into a $\psi(x, T)$ with infinitely many zero-crossings, each such zero corresponding to a critical zero of $\zeta(1/2 + ix)$. It is not yet known whether there are additional consequences of this observation. Some details are given in [77].

31. H. S. M. (Donald) Coxeter (1907–2003). The renowned Canadian geometer H. S. M. Coxeter passed away in late March 2003. Coxeter was known for making extensive use of physical models in his research. A portion of his collection is on display at the University of Toronto, where he worked for 67 years. The model shown in Figure 2.14 now resides at York University in Toronto. A sculpture of five touching spheres, by John Robinson, which was presented to Coxeter on his 90th birthday, is shown in Figure 2.15.

Among his numerous published books, Regular Complex Polytopes, for example, is lavishly illustrated with beautiful and often intricate
figures. He was a friend of Maurits C. Escher, the graphic artist. In a 1997 paper, Coxeter showed that Escher, despite knowing no mathematics, had achieved “mathematical perfection” in his etching “Circle Limit III.” “Escher did it by instinct,” Donald Coxeter noted, “I did it by trigonometry.”

His *Introduction to Geometry* was widely used as a text for university courses in geometry. The spirit of his work is perhaps best captured by a quote from Bertrand Russell that Coxeter includes in the preface to *Introduction to Geometry*:

> Mathematics, rightly viewed, possesses not only truth, but supreme beauty—a beauty cold and austere, without appeal to any part of our weaker nature, without the gorgeous trappings of painting or music, yet sublimely pure, and capable of a stern

![Donald Coxeter's own kaleidoscope (see Color Plate VII). Courtesy of Asia Weiss.](image-url)
This quote is doubly interesting given the fact that Russell may have been responsible for Coxeter pursuing a mathematical career, according to Arthur Sherk, the executor for Coxeter’s mathematics. Russell, who was a family friend, read a prize-winning essay on dimensionality that Coxeter wrote at age 16. He then told Coxeter’s father that his son was unusually gifted mathematically, and urged him to change the direction of Coxeter’s education.

Along this line, Robert Moody wrote the following, in a letter supporting Coxeter’s nomination to receive an honorary doctorate at York University in Toronto, Canada:

Modern science is often driven by fads and fashion, and mathematics is no exception. Coxeter’s style, I would say, is singularly unfashionable. He is guided, I think, almost completely by a profound sense of what is beautiful.

Two sculptures based on Coxeter’s work decorate the Fields Institute in Toronto. One, hanging from the ceiling, is a three-dimensional projection of a four-dimensional regular polytope whose 120 faces are dodecahedrons as shown in Figure 2.16 (see Color Plate III).

Coxeter’s fascination with geometry extended beyond the purely intellectual. For example, he was intrigued by the suggestion that Einstein’s brain exhibited unusual bilateral symmetry, which in part ac-
counted for his genius, and has made provision for his brain to be similarly examined.

David Mumford recently commented that Coxeter placed great value on working out the details of complicated explicit examples:

In my book, Coxeter has been one of the most important 20th century mathematicians—not because he started a new perspective, but because he deepened and extended so beautifully an older esthetic. The classical goal of geometry is the exploration and enumeration of geometric configurations of all kinds, their symmetries and the constructions relating them to each other. The goal is not especially to prove theorems but to discover these perfect objects and, in doing this, theorems are only a tool that imperfect humans need to reassure themselves that they have seen them correctly. This is a flower garden whose beauty has almost been forgotten in the 20th century rush to abstraction and generality. I share Coxeter’s love of this perspective, which
has deep roots in algebraic as well as Euclidean geometry. I always found the algebraic roots-and-weights approach to Lie groups arid unsatisfying until I found Coxeter’s work fleshing this out with a rich tapestry of examples. My own interest in explicit compactifications of the moduli space of Abelian varieties led me to wonderful parts of his work on explicit fundamental domains for quadratic forms modulo $\text{GL}_n(\mathbb{Z})$. In the 21st century, I think we see signs of a renewed appreciation of the significance of the classical geometry mode in mathematics, perhaps linked with having easily usable computational tools. I trust that this perspective will never die. [156]

A color illustration (see Color Plate VII) of the octahedral kaleidoscope Coxeter had built. Asia Weiss writes

The kaleidoscope was not built by Coxeter, but rather designed by him and made in a workshop in London, England I believe in the late 1920s. . . Two kaleidoscopes were made: octahedral and icosahedral. (As the tetrahedral group is a subgroup in the octahedral group, the tetrahedral kaleidoscope was not made.) We also have the icosahedral one; but this one is damaged and I did not have it repaired as yet. [192]

32. Math meets ice. Figure 2.17 (see Color Plate V) shows Helaman Ferguson’s Costa surface sculpture, which he entered in the International Snow Sculpture Championship held at Breckenridge, Colorado, January 19-24, 1999 [69]. This piece was entitled “Invisible Handshake,” because it is the space between two hands just before they clasp. Ferguson carved this piece with the assistance of Stan Wagon, Dan Schwalbe, Tomas Nemeth, and (posthumously) Alfred Gray. Here is Ferguson’s account:

I choose this negative Gaussian curvature geometric form specifically because of the material properties of snow. Snow with its fair compressive strength and poor tensile strength is a caricature of stone. But negative Gaussian curvature, even in snow, presents a fabric of saddle points everywhere. Each point of the surface is the keystone of a pair of principal arches. There were 14 other snow sculptures completed at the Breckenridge affair; a week later they all completely imploded in the heat wave. Our negative Gaussian curvature snow carving stood, retained its structure, sublimed, thinned, gracile. (Taken from http://www.helasculpt.com)

33. Mathematics of Ferguson’s sculptures. The quotient group corresponding to Ferguson’s “Eight-Fold Way” sculpture is a certain
subgroup of \( SL_2(Z) \), i.e., the set of invertible, unit-determinant \( 2 \times 2 \) matrices with integer entries. One particular subgroup of \( SL_2(Z) \) corresponds to a tessellation of the hyperbolic circle by 7-gons. This design is used as the tiled base of Ferguson’s “Eight-Fold Way,” which is at the Mathematical Sciences Research Institute in Berkeley, CA. Another subgroup has a fundamental domain of 24 seven-gons, which has identifications corresponding to the surface of the marble sculpture above the base.

Ferguson’s “Figure-Eight Knot Complement II” sculpture corresponds to a certain subgroup of index 12 in the Bianchii group, which is \( SL_2(Z[\omega_3]) \), where \( \omega_3 = (-1 + i\sqrt{3})/2 \) is a third root of unity. Let \( \Gamma \) denote the multiplicative group of \( 2 \times 2 \) matrices generated by the matrices

\[
\begin{bmatrix}
1 & 0 \\
0 & \omega_3
\end{bmatrix}
\text{ and }
\begin{bmatrix}
0 & -1 \\
1 & 0
\end{bmatrix}.
\] (2.40)

This \( \Gamma \) is the fundamental group of the figure-eight knot complement. The complement is the double quotient \( U_2 \backslash SL_2(C)/\Gamma \), where
U_2 is the group of unitary matrices (i.e., inverse is conjugate transpose) in C. The first quotient U_2/SL_2(C) is geometrically the three-dimensional hyperbolic space. This group Γ is an “arithmetic” subgroup of SL_2(C). The group SL_2(Z[ω_3]) is known as the Eisenstein integers, a ring of algebraic integers. The figure-eight knot is absolutely unique in this respect—there is no other knot with this double quotient possessing the discrete group arithmetic property. For further details of the group-theoretic structure of these objects, see [187].

34. Clausen’s function and the figure-eight knot complement volume. As we saw in Section 2.4, the volume of the figure-eight knot complement is given by Equation (2.14). That is,

$$V = \frac{2}{\sqrt{27}} \sum_{k=0}^{\infty} \left( -\frac{1}{27} \right)^k \left( \frac{9}{(6k+1)^2} - \frac{9}{(6k+2)^2} - \frac{12}{(6k+3)^2} - \frac{3}{(6k+4)^2} + \frac{1}{(6k+5)^2} \right).$$

(2.41)

The reason is sketched below. Note that this proof crucially requires knowing the answer in advance, and moving back from the discovered result to something provable.

(a) We take the log sine integral

$$V = -2 \int_0^{\pi/3} \log \left( 2 \sin \left( \frac{t}{2} \right) \right) dt$$

(2.42)

as the defining formula for the requisite volume. Recall that the Clausen function is given by

$$\text{Cl}_2(\theta) = \sum_{n>0} \frac{\sin(n\theta)}{n^2},$$

(2.43)

which satisfies \( \text{Cl}_2(\pi) = G \). Then integration of (2.42) shows

$$V = i \left\{ \text{Li}_2(e^{i\pi/3}) - \text{Li}_2(e^{-i\pi/3}) \right\}$$

$$= 2 \text{ImLi}_2 \left( \frac{1 + i\sqrt{3}}{2} \right) = 2 \text{Cl}_2 \left( \frac{\pi}{3} \right) = 3 \text{Cl}_2 \left( \frac{2\pi}{3} \right).$$

All the requisite details about Clausen’s function are to be found in Lewin [141].
(b) A hypergeometric equivalent formulation of (2.41) is

\[
\frac{V}{\sqrt{3}} = 2F \left( \frac{1}{6}, \frac{1}{6}, 1; \frac{7}{6}, \frac{7}{6}, -\frac{1}{27} \right) - \frac{1}{2} F \left( \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 1; \frac{4}{3}, \frac{4}{3}, -\frac{1}{27} \right)
\]

\[\quad - \frac{8}{27} F \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1; \frac{3}{2}, \frac{3}{2}, -\frac{1}{27} \right) - \frac{1}{24} F \left( \frac{2}{3}, \frac{2}{3}, 1; \frac{5}{3}, \frac{5}{3}, -\frac{1}{27} \right)
\]

\[\quad + \frac{2}{225} F \left( \frac{5}{6}, \frac{5}{6}, 1; \frac{11}{6}, \frac{11}{6}, -\frac{1}{27} \right)
\]

which with some effort is expressible in terms of the dilogarithm. This leads to the following:

\[
V \equiv \text{Im} \left\{ 4 \text{Li}_2 \left( \frac{i\sqrt{3}}{3} \right) - \frac{8}{3} \text{Li}_2 \left( \frac{i\sqrt{3}}{9} \right) + \text{Li}_2 \left( \frac{1}{2} - \frac{i\sqrt{3}}{6} \right) + 8 \text{Li}_2 \left( -\frac{1}{2} + \frac{i\sqrt{3}}{6} \right) \right\}
\]

(c) Now, Lewin in Equation (5.5) of [141] gives

\[
\text{Im} \text{Li}_2 \left( re^{i\theta} \right) = \omega \log(r) + \frac{1}{2} \text{Cl}_2 \left( 2\omega + 2\theta \right) + \frac{1}{2} \text{Cl}_2 \left( 2\theta \right),
\]

where \( \omega = \arctan(r \sin \theta / (1 - r \cos \theta)) \). Using this, a proof that (2.41) holds is reduced to showing that, with \( \alpha = \arctan(\sqrt{3}/9) \),

\[
4 \text{Cl}_2 \left( \frac{\pi}{3} \right) = 2 \text{Cl}_2 \left( 2\alpha \right) + \text{Cl}_2 \left( \pi + 2\alpha \right) - 3 \text{Cl}_2 \left( \frac{5}{3}\pi + 2\alpha \right),
\]

which is true by applying the two variable identities for Clausen’s function given in Equations (4.61) and (4.63) of [141], with \( \theta = \frac{\pi}{2} \).

(d) Many other identities lie in (4.63) such as, with \( \alpha = \arctan \left( \frac{1}{3} \right) \),

\[
6 \text{G} = 2 \text{Cl}_2 \left( 2\alpha \right) - 3 \text{Cl}_2 \left( 2\alpha - \frac{\pi}{2} \right) + \text{Cl}_2 \left( 2\alpha + \frac{\pi}{2} \right).
\]

A much harder identity is

\[
\frac{7\sqrt{7}}{4} L_{-\gamma} \left( 2 \right) = 3 \text{Cl}_2 \left( \alpha \right) - 3 \text{Cl}_2 \left( 2\alpha \right) + \text{Cl}_2 \left( 3\alpha \right)
\]

with \( \alpha = 2 \arctan \left( \sqrt{7} \right) \).
35. **Further identities for the knot complement volume.** These are explored below.

(a) On expanding the Clausen function of \((2.43)\), we obtain

\[
V = \sum_{n \geq 1} \frac{2 \sin(n\pi/3)}{n^2}
\]

\[
= \sqrt{3} \left( \sum_{n=0}^{\infty} \frac{1}{(6n+1)^2} + \sum_{n=0}^{\infty} \frac{1}{(6n+2)^2} - \sum_{n=0}^{\infty} \frac{1}{(6n+4)^2} - \sum_{n=0}^{\infty} \frac{1}{(6n+5)^2} \right),
\]

or equivalently,

\[
V = \frac{\sqrt{3}}{9} \sum_{n \geq 1} \frac{n - \frac{1}{2}}{(n - \frac{1}{2})^2(n - \frac{4}{3})^2}.
\]

(b) Changing variables in \((2.42)\) and using the binomial theorem, we derive

\[
V = -2 \int_0^1 \frac{\log(y)}{\sqrt{1 - (\frac{y}{2})^2}} dy = 2 \sum_{n=0}^{\infty} \frac{(2n)}{(2n+1)^2} 16^n.
\]

The next two equivalent identities are derivable using (1.76) in [141] which gives the series for \(\text{Li}_2(e^{i\pi/3})\):

(c)

\[
V = 2\pi/3 \left( 1 - \log\left(\frac{\pi}{3}\right) + \sum_{m \geq 1} \frac{\zeta(2m)}{m(2m+1)6^{2m}} \right),
\]

and

\[
V = 2\pi/3 - 2\pi/3 \log\left(\frac{\pi}{3}\right) + 2 \sum_{n \geq 1} \frac{B_n}{2n} \left(\frac{\pi}{3}\right)^{2n+1}.
\]

(d) Show that

\[
V = 2\sqrt{3} \text{Im} L_2 \left(\frac{i\sqrt{3} + 1}{2}\right) = -\sqrt{3} \int_0^1 \frac{\log(y)}{1 - y + y^2} dy.
\]
Hence expanding the last denominator and differentiating the $\beta$-function (see Section 5.4), deduce that

\[
V = 2 \sqrt{3} \sum_{n \geq 1} \frac{\Psi(n) - \Psi(2n)}{n(\binom{2n}{n})} = 2 \sqrt{3} \sum_{n \geq 1} \frac{\sum_{k=1}^{2n-1} \frac{1}{n}}{n(\binom{2n}{n})}
\]

(f) This is equivalent to

\[
V = 2 \sqrt{3} \int_0^{1/2} \frac{\log \left( \frac{1+s}{1-s} \right)}{(1 - s^2) \sqrt{1 - 4s^2}} ds - 2 \sqrt{3} \int_0^{1/2} \frac{\log \left( \frac{1-s^2}{1-s} \right)}{(1 - s^2) \sqrt{1 - 4s^2}} ds,
\]

where the first integral corresponds to $\sum_{k=1}^{2n-1} 1/k$ and the second to $\sum_{k=1}^{2n-1} 1/k$. These are equivalent to

\[
V = \sqrt{3} \int_0^{\pi/2} \log \left( \frac{1 + \sin t / 2}{1 - \sin^2 t / 4} \right) \frac{1}{1 - \sin^2 t / 4} dt,
\]

where $\int_0^{\pi/2} \frac{\log \left( \frac{1 + \sin t / 2}{1 - \sin^2 t / 4} \right)}{(1 - \sin^2 t / 4)} dt = \Gamma^2(N+1)/\Gamma(2N+2)$, and $\int_0^{\pi/2} \frac{\log \left( \frac{1 + \sin t / 2}{1 - \sin^2 t / 4} \right)}{(1 - \sin^2 t / 4)} dt = \Gamma^2(N+1/2)/\Gamma(2N+1)$. A symmetric rendition of the integral is:

\[
V = 2 \sqrt{3} \int_0^{1/2} \frac{(1+s) \log (1+s) - (1-s) \log (1-s)}{(1 - s^2) \sqrt{1 - 4s^2}} ds.
\]

(g) Deduce that

\[
V = \sqrt{3} \sum_{n=0}^{\infty} \frac{\sum_{k=1}^{2n+1} (-1)^{k+1} k^{-1}}{n(\binom{2n}{n}) (2n+1)}.
\]

(h) Finally,

\[
-\sqrt{3} \sum_{n=2}^{\infty} \frac{\sum_{k=1}^{n-1} k^{-1}}{n(\binom{2n}{n})} = \frac{\sqrt{3}}{2} \int_0^1 \frac{\log (1 - t (1-t))}{1 - t + t^2} dt.
\]
2.10. Commentary and Additional Examples

Let
\[ H_1 = \sum_{n=1}^{\infty} \frac{\sum_{k=1}^{n-1} k^{-1}}{n \binom{2n}{n}}, \quad H_2 = \sum_{n=1}^{\infty} \frac{\sum_{k=1}^{2n-1} k^{-1}}{n \binom{2n}{n}}. \]

Then \( V = 2 \sqrt{3} \{ H_2 - H_1 \} \) and, following the logic of the previous exercise,

\[
H_1 = \sum_{k=0}^{\infty} \left(\frac{-1}{27}\right)^k \left\{ -\frac{1/3}{(6k+1)^2} - \frac{1}{(6k+2)^2} + \frac{10/9}{(6k+3)^2} 
+ \frac{1/3}{(6k+4)^2} - \frac{1/27}{(6k+5)^2} \right\},
\]

while

\[
H_2 = \sum_{k=0}^{\infty} \left(\frac{-1}{27}\right)^k \left\{ \frac{2/3}{(6k+1)^2} - \frac{2/9}{(6k+3)^2} - \frac{2/27}{(6k+5)^2} \right\}.
\]

See [141] for additional details.

36. Census of hyperbolic knots. The URL [http://newweb.cecm.sfu.ca/cgi-bin/KnotPlot/objtest/hyperbolic_census?knot=k4.1](http://newweb.cecm.sfu.ca/cgi-bin/KnotPlot/objtest/hyperbolic_census?knot=k4.1) contains a census of hyperbolic knots (most, but not all, knots are hyperbolic). The figure-eight knot, not the trefoil, is now simplest when viewed by the number of perfect tetrahedra in its complement.

37. Jeff Weeks on experimental topology. Jeff Weeks recently wrote:

There are plenty of such [experimentally discovered topology] results, but most would require a fair amount of explanation to be significant to non-specialists. For example, one of my favorites is the (computationally discovered!) pattern in the canonical triangulation for two-bridge knot and link complements. The canonical triangulation is geometrically defined, yet it exactly encodes the twists in the (topological) tangle decomposition of the knot or link. The correspondence is remarkably simple, with exactly two tetrahedra realizing each twist. This result has since been proved, but the proof is long and difficult. ... I could try to dig up a figure illustrating how the pairs of tetrahedra realize the twists, ... but then it’s not clear that you could explain it easily so that a non-specialist would understand why it’s such an amazingly beautiful thing (as opposed to the reader struggling just to get a dim grasp of what the result is saying, without really appreciating what makes it cool).
38. **Griffeath’s “psoup” cellular automata web site.** David Griffeath well describes his site [http://psoup.math.wisc.edu](http://psoup.math.wisc.edu) as follows:

Hi there. I’m a math prof at the University of Wisconsin-Madison whose research these days focuses on self-organization of random cellular automata. For the past ten years or so I have been producing colorful computer graphics and animations that illustrate the ability of local parallel update rules to generate spatial structure from disordered initial states. My work has appeared in numerous books and periodicals, including *Nonlinear Science Today* and *Scientific American*. Some of my cellular automaton (CA) rules have been featured in the simulation packages CA-LAB and James Gleick’s *Chaos: The Software*. This home page is intended to provide a gallery of my images and movies, as well as links to software that allows you to design your own.

It’s tempting to think of self-organization as evolution from primordial soup. Machines that orchestrate such dynamics are sometimes called mixmasters. I use both garden-variety PCs and dedicated Cellular Automaton Machines (CAMs) as mixmasters. Since my other great fixation in life is gastronomy (witness the important 3-letter word hidden in my Welsh last
39. Fractal cards. Not all impressive representations require a computer. Elaine Simmt and Brent Davis [180] describe lovely constructions made by repeated paper folding and cutting that result in beautiful fractal “pop-up” cards. Nonetheless, in Figure 2.19, we show the seventh iterate of a Sierpinski triangle built in software by following those paper cutting and folding rules in software. Note the similarity to the tetrahedron in Figure 2.1. Recursive Maple code is given below:

```maple
sierpinski:= proc(n::nonnegint)
local p1, p2, q1, q2, r1, r2, plotout;
p1:= [1.,0.,0.]; q1:= [-1.,0.,0.]; r1:= [0.,0.,1.];
p2:= [1.,1.,0.]; q2:= [-1.,1.,0.]; r2:= [0.,1.,1.];
plotout:= polys(n, p1, p2, r1, r2, q1, q2);
return PLOT3D( plotout, SCALING(CONSTRAINED),
AXESSTYLE(NONE), STYLE(PATCHNOGRID), ORIENTATION(90,45) );
end:
```

Figure 2.19. 7th iterate of Sierpinski triangle made by paper cutting and folding.
polys:= proc( n::nonnegint, p1, p3, r1, r3, q1, q3 )
local p2, q2, r2, s1, s2, s3, t1, t2, t3, u2, u3;
if n=0 then return POLYGONS([p1,p3,r3,r1], [q1,q3,r3,r1]) fi;
p2:= (p1+p3)/2; q2:= (q1+q3)/2; r2:= (r1+r3)/2;
s1:= (p1+r1)/2; s2:= (p2+r2)/2; s3:= (p3+r3)/2;
t1:= (q1+r1)/2; t2:= (q2+r2)/2; t3:= (q3+r3)/2;
u2:= (p2+q2)/2; u3:= (p3+q3)/2;
return polys(n-1, p2, p3, s2, s3, u2, u3),
polys(n-1, s1, s2, r1, r2, t1, t2),
polys(n-1, u2, u3, t2, t3, q2, q3),
POLYGONS([p1,p2,s2,s1], [q1,q2,t2,t1]); end:

40. Gauss on learning. In Boris Stoicheff’s often enthralling biography of Gerhard Herzberg (1903-1999), Gauss is recorded as writing

It is not knowledge, but the act of learning, not possession but the act of getting there which generates the greatest satisfaction.

[183, page 42]

Herzberg, who fled Germany for Saskatchewan in 1935, won the 1971 Nobel Prize in Chemistry for his pioneering work in molecular spectroscopy. His impact on Canadian—and international—science, signalized in chemistry, physics and astronomy, has been enormous.

41. Horizontal Riemann curves. Figure 2.20 plots the modulus of the function $Z$ defined by $(x, y) \mapsto |\zeta(x+iy)|$ for $1/5 < x < 4/5$ and $1 < y < 100$. Much related material and many illustrations are to be found in Brian Conrey’s survey [72].

Plot $Z(x, y)$ as a function of $x$ on the critical strip $[0, 1]$ for various values of $y$. (Compare what happens with the roles of $x$ and $y$ reversed.) As it turns out, the monotonicity exhibited in the graph of level curves of $Z(x, y)$ implies the Riemann Hypothesis. This conclusion is given in [198], and was discovered while the first author of that paper was teaching an undergraduate complex variable class.

42. Hardy and Littlewood’s Four Axioms for Collaboration. Harald Bohr, quoting from the preface of Béla Bollobás’ 1988 edition of Littlewood’s Miscellany, said:

The first [axiom] said that when one wrote to the other (they often preferred to exchange thoughts in writing instead of orally), it was completely indifferent whether what they said was right or wrong. As Hardy put it, otherwise they could not write completely as they pleased, but would have to feel a certain responsibility thereby. The second axiom was to the effect that,
when one received a letter from the other, he was under no obligation whatsoever to read it, let alone answer it—because, as they said, it might be that the recipient of the letter would prefer not to work at that particular time, or perhaps that he was just then interested in other problems. ... The third axiom was to the effect that, although it did not really matter if they both thought about the same detail, still, it was preferable that they should not do so. And, finally, the fourth, and perhaps most important axiom, stated that it was quite indifferent if one of them had not contributed the least bit to the contents of a paper under their common name; otherwise there would constantly arise quarrels and difficulties in that now one, and now the other, would oppose being named co-author.

These rules work very well in the present age.

43. **What is a tool?** James O’Donnell wrote a mere five years ago:

> I am a student of the works of St. Augustine and shall begin accordingly with confession. The single most transforming feature of cyberspace as we inhabit it in 1997 for my own scholarship can be found in a warehouse on the edges of downtown Seattle.

> I mean the nerve center of www.amazon.com. [160]

Google, MathSciNet—the online version of Mathematical Reviews at [http://e-math.ams.org/mathscinet](http://e-math.ams.org/mathscinet), and Amazon.com are just as much tools of discovery as are PSLQ, the Inverse Calculator and Mathematica.


> Three years ago, said Dr. Zanelli in Chile, one of his own students posted a paper and the next day received an e-mail message from Dr. Witten. The student was at first so shocked that he accused Dr. Zanelli of playing an elaborate practical joke.

> “We learned that great physicists do read the archives daily and they browse through all the preprints,” Dr. Zanelli said, “even if they come from an obscure place in the end of the world.”

> Dr. Witten’s instant response, Dr. Zanelli said, “was like having the pope drop by for tea.”

Such is the promise of the wired world, deluges of spam not withstanding.
45. **False proofs of big theorems.** David Einstein has commented that in the last generation, there has always been at least one somewhat serious purported proof of the Poincaré conjecture under scrutiny. Similar comments hold for Fermat’s Last Theorem, the Riemann Hypothesis, the Four Color Theorem, and so on. Many famous mathematicians have survived premature publicity for proofs found later to be unavoidably flawed. Hans Rademacher’s putative proof of the falsehood of the Riemann Hypothesis made the pages of *Time* in the late forties, even after the flaw had been discovered by Siegel.\(^7\)

Of course, even the existence of generally accepted proofs does not discourage many amateurs from hunting for counterexamples nor from trying to square the circle or trisect angles.

46. **Research, teaching and communication.** The Fields medalist Bill Thurston, in his 1995 article, “On proof and progress,” makes the observation about researchers’ habits that

> Mathematicians have developed habits of communication that are often dysfunctional. Organizers of colloquium talks everywhere exhort speakers to explain things in elementary terms. Nonetheless, most of the audience at an average colloquium talk gets little of value from it. Perhaps they are lost within the first 5 minutes, yet sit silently through the remaining 55 minutes. Or perhaps they quickly lose interest because the speaker plunges into technical details without presenting any reason to investigate them. At the end of the talk, the few mathematicians who are close to the field of the speaker ask a question or two to avoid embarrassment.

This pattern is similar to what often holds in classrooms, where we go through the motions of saying for the record what we think the students “ought” to learn, while the students are trying to grapple with the more fundamental issues of learning our language and guessing at our mental models. Books compensate by giving samples of how to solve every type of homework problem. Professors compensate by giving homework and tests that are much easier than the material “covered” in the course, and then grading the homework and tests on a scale that requires little understanding. We assume that the problem is with the students rather than with communication: that the students either just don’t have what it takes, or else just don’t care.

Outsiders are amazed at this phenomenon, but within the mathematical community, we dismiss it with shrugs.
47. **Riemann and robust notation.** Figures [2.7 and 2.8](#) which reproduce the first two pages of the final manuscript of Riemann’s celebrated 1859 paper [172](#) illustrate how robust mathematical notation is. If a counter-example or theorem is originally due to Hilbert or Cauchy, there is a good chance we reproduce it with exactly the same syntax.

48. **Hoffman’s art.** Experimental visualization in low-dimensional geometry was one of the primary motivations for Klaus Peters’ decision in the early nineties to establish the journal *Experimental Mathematics*—see [http://www.expmath.org](http://www.expmath.org). This is now a flourishing, high quality journal with several Fields medalists on its board. Some of the better examples of geometric visualization are due to David Hoffman—see the web sites [http://www.gang.umass.edu](http://www.gang.umass.edu) and [http://emsh.calarts.edu/~mathart/portfolio/](http://emsh.calarts.edu/~mathart/portfolio/). SPD_Costa_portfolio.html

49. **Euler, Goldbach and the birth of $\zeta$.** What follows is a direct transcription of correspondence between Euler and Goldbach [123](#), leading to the origin of the zeta function and multi-zeta values.


[... ] Als ich neulich die vermeinten summas der beiden letzeren serierum in meinem vorigen Schreiben wieder betrachtet, habe ich alsofort wahrgenommen, daß selbige aus einem bloßem Schreibfehler entstanden, von welchem es aber in der Tat heißet: Si non errasset, fecerat ille minus.$^3$

denn ich bin durch diese Gelegenheit auf summationes aliarum serierum geraten, die ich sonst kaum gesucht, viel weniger gefunden haben würde.

Ich halte dafür, daß es ein problema problematum ist, die summam huius:

\[
\sum_{n=1}^{\infty} \frac{1}{n^2} = 1 + \frac{1}{2^2} + \frac{1}{3^2} + \frac{1}{4^2} + \ldots
\]

in den casibus zu finden, wo $m$ et $n$ nicht numeri integri pares et sibi aequales sind, doch gibt es casus, da die summa angegeben werden kann, exempli gr[atia], si $m = 1$, $n = 3$, denn es ist

\[
1 + \frac{1}{2^2} + \frac{1}{3^2} + \frac{1}{4^2} + \ldots = \pi^2.
\]

---

$^3$Frei zitiert nach Marcus Valerius Martialis, I, 21,9
(wenn π gewöhnlichermaßen für die peripheriam circuli, cuius diameter = 1, genommen wird), hingegen wieß ich die summas serierum

\[ A \cdots 1 + \frac{1}{2^2} \left(1 + \frac{1}{2}\right) + \frac{1}{3^2} \left(1 + \frac{1}{2} + \frac{1}{3}\right) + \frac{1}{4^2} \left(1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4}\right) + \text{etc.} \]

\[ B \cdots 1 + \frac{1}{2^3} \left(1 + \frac{1}{2}\right) + \frac{1}{3^3} \left(1 + \frac{1}{2} + \frac{1}{3}\right) + \frac{1}{4^3} \left(1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4}\right) + \text{etc.} \]

noch nicht, ob ich gleich weiß, daß \[ 2A + B = \frac{19\pi^6}{2^5 \times 3^2}, \]
wie ich denn auch die summam der folgenden beiden /55/ serierum C + D allezeit finden kann, si \( m \) et \( n \) sint numeri quicunque

\[ C \cdots 1 + \frac{1}{2^m} \left(1 + \frac{1}{2^m}\right) + \frac{1}{3^n} \left(1 + \frac{1}{2^m} + \frac{1}{3^n}\right) + \text{etc.} \]

\[ D \cdots 1 + \frac{1}{2^m} \left(1 + \frac{1}{2^m}\right) + \frac{1}{3^n} \left(1 + \frac{1}{2^m} + \frac{1}{3^n}\right) + \text{etc.} \]

Übrigens beziehe ich mich auf mein voriges Schreiben und verbleibe nächst herzlicher Anwünschung eines glücklichen neuen Jahres[...]

(b) “Lisez Euler, lisez Euler, c’est notre maître a tous.” [86]

This letter is the first in which Goldbach precisely formulates the series which sparked Euler’s further investigations into what would become known as the Zeta-function. These investigations were apparently due to a serendipitous mistake. The first sentence above translates as follows:

When I recently considered further the indicated sums of the last two series in my previous letter, I realized immediately that the same series arose due to a mere writing error, from which indeed the saying goes, “Had one not erred, one would have achieved less.” (Si non errasset, fecerat ille minus). [Translation thanks to Martin Matmüller, scientific collaborator of Euler’s Opera Omnia, vol. IVA4, Birkhäuser Verlag.]

(c) Confirm Goldbach’s evaluation (\( m = 3, n = 1 \)):

\[ \zeta(3, 1) + \zeta(4) = \frac{\pi^4}{72} \]

(in the language of Section 3.4 of the second volume of this work).

50. Gauss: the next generation.
2.10. Commentary and Additional Examples

Gauss’s second son, Eugene, emigrated to the United States in 1830, enlisted in the army, and later went into business in Missouri. Eugene is said to have had some of his father’s gift for languages and the ability to perform prodigious arithmetic calculations, which he did for recreation after his sight failed him in old age. (David T. Lykken [143])

51. Flexibility.

When the facts change, I change my mind. What do you do, sir? (John Maynard Keynes, quoted in The Economist, Dec. 18, 1999, pg. 47)

52. Mathematics and the aesthetic impulse.

If my teachers had begun by telling me that mathematics was pure play with presuppositions, and wholly in the air, I might have become a good mathematician, because I am happy enough in the realm of essence. But they were overworked drudges, and I was largely inattentive, and inclined lazily to attribute to incapacity in myself or to a literary temperament that dullness which perhaps was due simply to lack of initiation. (George Santayana, Persons and Places [178 pg. 238–9])
Figure 2.20. The modulus of the zeta function.
I am ashamed to tell you to how many figures I carried these com-
putations, having no other business at the time.

– Issac Newton, personal journal, 1666

The desire, as well as the need, to calculate ever more accurate values of
\( \pi \), the ratio of the circumference of a circle to its diameter, has challenged
mathematicians for many centuries. In recent years, \( \pi \) computations have
provided some fascinating examples of computational mathematics. But
first, a little historical background, which we have condensed from a 1997
article [17]. Additional historical details are available from the fascinating
new book *Pi Unleashed* [7], and from [49] [34]. We should also mention
the MacTutor web site, maintained by the Department of Mathematics
at the University of St. Andrews in Scotland: [http://www-gap.dcs.st-
and.ac.uk/~history](http://www-gap.dcs.st-and.ac.uk/~history) This is particularly good for biographical information
about historical mathematicians, including those involved with \( \pi \).

### 3.1 A Short History of Pi

About 2000 BCE, the Babylonians used the approximation \( 3\frac{1}{8} = 3.125 \).
At this same time or earlier, according to an ancient Egyptian document,
Egyptians assumed that a circle with diameter nine has the same area as a
square of side eight, which implies \( \pi = \frac{256}{81} = 3.1604 \ldots \) Some have argued
from the following biblical passage that the ancient Hebrews used \( \pi = 3 \):

> Also, he made a molten sea of ten cubits from brim to brim, round
> in compass, and five cubits the height thereof; and a line of thirty
cubits did compass it round about (1 Kings 7:23; see also 2 Chron.
4:2).

The first rigorous mathematical calculation of the value of \( \pi \) was due
to Archimedes (ca. 250 BCE), who used a scheme based on inscribed
and circumscribed polygons to obtain the bounds \( 3\frac{10}{71} < \pi < 3\frac{1}{7} \). Indeed,
Archimedes’ scheme constitutes the first true algorithm for \( \pi \), in the sense that it is a well-defined scheme that is capable of producing an arbitrarily accurate value for the constant. This scheme can be stated as a simple recursion, as follows. Set \( a_0 = 2\sqrt{3} \) and \( b_0 = 3 \). Then define

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

This recursion converges to \( \pi \), with the error decreasing by a factor of approximately four with each iteration. Variations of Archimedes’ geometrical scheme were the basis for all high-accuracy calculations of \( \pi \) for the next 1,800 years. For example, the Chinese mathematician Tsu Chung-Chih used a variation of this method to compute \( \pi \) correct to seven digits in the fifth century CE.

Little progress was made in Europe during the dark ages, but one very significant advance in arithmetic was made in India. This was the invention, in about 450 CE, of our modern positional, zero-based decimal arithmetic system—the Indo-Arabic system. This discovery greatly accelerated arithmetic in general, and computing \( \pi \) in particular. The Indo-Arabic system was introduced into Europe in 1000 CE, but due to resistance from several quarters, centuries elapsed before it finally enjoyed widespread use. The resistance ranged from accountants who didn’t want their livelihood upset to clerics who regarded the system as “diabolical,” on account of what they incorrectly assumed was its origin in the Arabic world. European commerce resisted the system until the 18th century, and even in scientific circles, its usage was limited until the 17th century [118]. The difficulty of doing arithmetic prior to the Indo-Arabic system is indicated by the words of counsel given to a wealthy German merchant in the 16th century, who was considering where to send his son for college:

If you only want him to be able to cope with addition and subtraction, then any French or German university will do. But if you are intent on your son going on to multiplication and division—assuming that he has sufficient gifts—then you will have to send him to Italy. [118, pg. 577]

In the 17th century, Newton and Leibniz discovered calculus, and this powerful new tool was quickly exploited to find new formulas for \( \pi \). One early calculus-based formula comes from the integral

\[
\arctan x = \int_0^x \frac{dt}{1 + t^2} = \int_0^x (1 - t^2 + t^4 - t^6 + \cdots) dt = x - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} + \frac{x^9}{9} - \cdots.
\]
3.1. A Short History of Pi

Substituting \( x = 1 \) gives the well-known Gregory–Leibniz formula
\[
\pi/4 = 1 - 1/3 + 1/5 - 1/7 + 1/9 - 1/11 + \cdots
\] (3.3)
(recall our discussion of Gregory’s series in Section 2.2). This particular series is practically useless for computing \( \pi \)—it converges so slowly that hundreds of terms would be required to compute even two correct digits. However, by employing a trigonometric identity
\[
\pi/4 = \arctan(1/2) + \arctan(1/3),
\] (3.4)
attributed to Euler in 1738, you can obtain
\[
\begin{align*}
\pi/4 &= \frac{1}{2} - \frac{1}{3\cdot2^3} + \frac{1}{5\cdot2^5} - \frac{1}{7\cdot2^7} + \cdots \\
&+ \frac{1}{3} - \frac{1}{3\cdot3^3} + \frac{1}{5\cdot3^5} - \frac{1}{7\cdot3^7} + \cdots,
\end{align*}
\] (3.5)
which converges much more rapidly. An even faster formula, discovered a generation earlier by Machin, can be obtained using the identity
\[
\pi/4 = 4\arctan(1/5) - \arctan(1/239)
\] (3.6)
in a similar way. This formula was used in numerous computations of \( \pi \), culminating with Shanks’ computation of \( \pi \) to 707 decimal digits accuracy in 1874 (although it was later found that this result was in error after the 527th decimal place).

Newton himself discovered a different formula. He began by considering the area \( A \) of the left-most region under the circle as shown in Figure 3.1. On one hand, this is merely the difference between the area of the circular sector, which is \( \pi/24 \), and the area of the triangle, which is \( \sqrt{3}/32 \). On the other hand, \( A \) can be written as the integral
\[
A = \int_{0}^{1/4} \sqrt{x-x^2} \, dx.
\] (3.7)
By employing his own binomial theorem, Newton wrote (3.7) as:
\[
\begin{align*}
A &= \int_{0}^{1/4} x^{1/2}(1 - x)^{1/2} \, dx \\
&= \int_{0}^{1/4} x^{1/2} \left(1 - x/2 - x^2/8 - x^3/16 - 5x^4/128 - \cdots\right) \, dx \\
&= \int_{0}^{1/4} \left(x^{1/2} - \frac{x^{3/2}}{2} - \frac{x^{5/2}}{8} - \frac{x^{7/2}}{16} - \frac{5x^{9/2}}{128} - \cdots\right) \, dx.
\end{align*}
\] (3.8)
Integrating this series term-by-term and combining the above results yielded the formula
\[
\pi = \frac{3\sqrt{3}}{4} + 2\left(\frac{1}{3 \cdot 8} - \frac{1}{5 \cdot 32} - \frac{1}{7 \cdot 128} - \frac{1}{9 \cdot 512} - \cdots\right). \quad (3.9)
\]
Newton personally used this formula to compute \(\pi\). He recorded 15 digits in his diary, but as he later confessed, “I am ashamed to tell you to how many figures I carried these computations, having no other business at the time.”

One of the more interesting figures in the history of \(\pi\) calculations is Johan Zacharias Dase, who lived in Vienna in the mid-1800s. According to the MacTutor web site (see above), Dase once demonstrated his computational skill by multiplying \(79532853 \times 93758479 = 7456879327810587\) in just 54 seconds; two 20-digit numbers required 6 minutes; two 40-digit numbers required 40 minutes; two 100-digit numbers required 8 hours 45 minutes. After being shown how to use the formula
\[
\frac{\pi}{4} = \arctan(1/2) + \arctan(1/5) + \arctan(1/8), \quad (3.10)
\]
he calculated \(\pi\) to 200 places in his head. He later calculated a seven-digit logarithm table, and extended a table of integer factorizations to 10,000,000. Gauss requested that Dase be permitted to assist him, but Dase died shortly afterward.

Along this line, recent historical research has uncovered several non-European mathematicians who did notable early work on \(\pi\) that until
3.1. A Short History of Pi

recently was not well known. For example, the Chinese mathematician Tsu Chung-Chih used a variation of Archimedes’ method to compute \( \pi \) correct to seven digits in the fifth century. A millennium later Al-Kăšī in Samarkand, “who could calculate as eagles can fly,” computed \( 2\pi \) in sexagecimal as

\[
6 + \frac{16}{60} + \frac{59}{60^2} + \frac{28}{60^3} + \frac{01}{60^4} + \frac{34}{60^5} + \frac{51}{60^6} + \frac{46}{60^7} + \frac{14}{60^8} + \frac{50}{60^9}
\]

(accurate to seventeen decimal places) using \( 3 \cdot 2^{28} \)-gons. Another remarkable but little-known mathematician was Madhava of Sangamagramma, who lived in India in the late 1300s and early 1400s. Madhava derived the Gregory-Leibniz series for \( \pi \) (3.3) at least 200 years before Gregory or Leibniz found it. He also derived the variant series

\[
\pi = \sqrt{12} \left( 1 - \frac{1}{3 \cdot 3} + \frac{1}{5 \cdot 3^2} - \frac{1}{7 \cdot 3^3} + \cdots \right),
\]

and used it to compute \( \pi \) to 11 decimal places. For additional information, see [34] and the MacTutor web site.

One motivation for computations of \( \pi \) was very much in the spirit of modern experimental mathematics: to see if the decimal expansion of \( \pi \) repeats, which would mean that \( \pi \) is the ratio of two integers (i.e., rational), or to recognize \( \pi \) as some algebraic constant. The question of the rationality of \( \pi \) was settled in the late 1700s, when Lambert and Legendre proved that the constant is irrational. The question of whether \( \pi \) is algebraic was settled in 1882, when Lindemann proved that it is transcendental. Lindemann’s proof also settled, once and for all, the ancient Greek question of whether the circle could be squared with ruler and compass: It cannot, because numbers that are the lengths of lines that can be constructed using ruler and compasses (often called constructible numbers) are necessarily algebraic, and squaring the circle is equivalent to constructing the value \( \pi \).

In 1945, Ferguson utilized some mechanical calculating machines to compute \( \pi \) to 530 decimal digits, using the formula

\[
\frac{\pi}{4} = 3 \arctan \left( \frac{1}{4} \right) + \arctan \left( \frac{1}{20} \right) + \arctan \left( \frac{1}{1985} \right),
\]

and over the next two years increased this to 808 digits. With this result, they discovered that Shanks’ 1874 computation was wrong after the first 527 places.

While such devices saved considerable labor compared with pencil-and-paper arithmetic, they were still a far cry from modern high-speed computers—each operand had to be manually typed, for example. The
first truly electronic computation of $\pi$ was performed in 1949 on the original ENIAC. This calculation was suggested by John von Neumann, who wished to study the digits of $\pi$ and $e$. Computing 2037 decimal places of $\pi$ on the ENIAC required 70 hours. A similar calculation today could be performed in a fraction of second on a personal computer.

Later computer calculations were further accelerated by the discovery of advanced algorithms for performing the required high-precision arithmetic operations. For example, in 1965 it was found that the newly-discovered fast Fourier transform (FFT) could be used to perform high-precision multiplications much more rapidly than conventional schemes. These methods dramatically lowered the computer time required for computing $\pi$ and other mathematical constants to high precision. These techniques will be discussed more in Section 6.2. See also [10] and [57].

In spite of these advances, until the 1970s all computer evaluations of $\pi$ still employed classical formulas, usually one of the Machin-type formulas. Some new infinite series formulas were discovered by Ramanujan around 1910, but these were not well known until quite recently when his writings were widely published. Ramanujan’s related mathematics may be followed in [108, 50, 36]. One of these series is the remarkable formula

$$\frac{1}{\pi} = \frac{2\sqrt{2}}{9801} \sum_{k=0}^{\infty} \frac{(4k)!}{(k!)^4} \frac{1103 + 26390k}{3964k^2}.$$ (3.13)

Each term of this series produces an additional eight correct digits in the result. Gosper used this formula to compute 17 million digits of $\pi$ in 1985. Gosper also computed the first 17 million terms of the continued fraction expansion of $\pi$. Figure 3.2 is a reproduction of a first day issue stamp commemorating the 75th birthday of Ramanujan. It was mailed from India with the correct postage added on the back. It arrived safely in Scotland despite the address being David Borwein’s home address.

At about the same time, David and Gregory Chudnovsky found the following variation of Ramanujan’s formula:

$$\frac{1}{\pi} = 12 \sum_{k=0}^{\infty} \frac{(-1)^k (6k)! (13591409 + 545140134k)}{(3k)! (k!)^3 640320^3 k + 3/2}. \quad (3.14)$$

Each term of this series produces an additional 14 correct digits. The Chudnovskys implemented this formula using a clever scheme that enabled them to utilize the results of an initial level of precision to extend the calculation to even higher precision. They used this method in several large calculations of $\pi$, culminating with a computation to over four billion decimal digits in 1994.
3.1. A Short History of Pi

Along this line, it is interesting to note that the Ramanujan-type series (see [49], pg. 188)

\[
\frac{1}{\pi} = \sum_{n=0}^{\infty} \left( \frac{2n}{16^n} \right)^3 \frac{42n + 5}{16}
\]  

(3.15)

permits one to compute the billionth binary digit of \(1/\pi\) without computing the first half of the series.

While the Ramanujan and Chudnovsky series are considerably more efficient than the classical formulas, they share with them the property that the number of terms one must compute increases linearly with the number of digits desired in the result. In other words, if you want to compute \(\pi\) to twice as many digits, you have to evaluate twice as many terms of the series.

In 1976, Eugene Salamin and Richard Brent independently discovered an algorithm for \(\pi\) based on the arithmetic-geometric mean (AGM) and some ideas originally due to Gauss in the 1800s (although for some reason Gauss never saw the connection to computing \(\pi\)). The Salamin–Brent algorithm may be stated as follows. Set \(a_0 = 1, b_0 = 1/\sqrt{2}\) and \(s_0 = 1/2\).
Calculate
\[ a_k = \frac{a_{k-1} + b_{k-1}}{2} \]
\[ b_k = \sqrt{a_{k-1}b_{k-1}} \]
\[ c_k = a_k^2 - b_k^2 \]
\[ s_k = s_{k-1} - 2^k c_k \]
\[ p_k = \frac{2a_k^2}{s_k}. \]

Then \( p_k \) converges **quadratically** to \( \pi \): Each iteration of this algorithm approximately doubles the number of correct digits—successive iterations produce 1, 4, 9, 20, 42, 85, 173, 347, and 697 correct decimal digits of \( \pi \). Twenty-five iterations are sufficient to compute \( \pi \) to over 45 million decimal digit accuracy. However, each of these iterations must be performed using a level of numeric precision that is at least as high as that desired for the final result.

Beginning in 1985, one of the present authors (Jonathan Borwein) and his brother Peter Borwein discovered some additional algorithms of this type [49]. One is as follows. Set \( a_0 = 1/3 \) and \( s_0 = (\sqrt{3} - 1)/2 \). Iterate
\[ r_{k+1} = \frac{3}{1 + 2(1 - s_k^3)^{1/3}} \]
\[ s_{k+1} = \frac{r_{k+1} - 1}{2} \]
\[ a_{k+1} = r_{k+1}^2 a_k - 3^k (r_{k+1}^2 - 1). \]

Then \( 1/a_k \) converges **cubically** to \( \pi \)—each iteration approximately triples the number of correct digits. Another algorithm is as follows: Set \( a_0 = 6 - 4\sqrt{2} \) and \( y_0 = \sqrt{2} - 1 \). Iterate
\[ y_{k+1} = \frac{1 - (1 - y_k^4)^{1/4}}{1 + (1 - y_k^4)^{1/4}} \]
\[ a_{k+1} = a_k (1 + y_{k+1})^4 - 2^{2k+3} y_{k+1} (1 + y_{k+1} + y_{k+1}^2). \]

Then \( a_k \) converges **quartically** to \( 1/\pi \). This particular algorithm, together with the Salamin–Brent scheme, has been employed by Yasumasa Kanada of the University of Tokyo in several computations of \( \pi \) over the past 15 years or so, including his 1999 computation of \( \pi \) to more than 206 billion decimal digits.

Daniel Shanks, who in 1961 computed \( \pi \) to over 100,000 digits, once declared that a billion digit computation would be “forever impossible.” But
both Kanada and the Chudnovskys computed more than one billion digits in 1989. Similarly, the intuitionist mathematicians Brouwer and Heyting once asserted the “impossibility” of ever knowing whether the sequence “0123456789” appears in the decimal expansion of $\pi$ [115]. This sequence was found in 1997 by Kanada, beginning at position 17,387,594,880. Even as late as 1989, British mathematical physicist Roger Penrose ventured, in the first edition of his book The Emperor’s New Mind, that we are not likely to know whether a string of ten consecutive sevens occurs in the decimal expansion of $\pi$ [163], pg. 115. By the time his book was published, Kanada had already found a string of ten consecutive sixes in his 480-million-digit computation of $\pi$. When one of the present authors mentioned this to Penrose in 1990, he replied that he was “startled to learn how far the combination of human mathematical ingenuity with computer technology has enabled the calculation of the decimal expansion of $\pi$ to be carried out.” Accordingly, he changed his text to “twenty consecutive sevens,” which appeared in subsequent printings of the book. This was just in time, as a string of ten consecutive sevens was found by Kanada in 1997, beginning at position 22,869,046,249.

As this book was nearing completion (2003), the authors learned that Kanada, with a team consisting of Y. Ushiro of Hitachi, H. Kuroda, and M. Kudoh of the University of Tokyo, and the assistance of nine others from Hitachi, have now computed $\pi$ to over 1.24 trillion decimal digits. Kanada and his team first computed $\pi$ in hexadecimal (base 16) to 1,030,700,000,000 places, using the following two arctangent relations for $\pi$:

\[
\begin{align*}
\pi &= 48 \arctan \frac{1}{49} + 128 \arctan \frac{1}{57} - 20 \arctan \frac{1}{239} + 48 \arctan \frac{1}{110443} \\
\pi &= 176 \arctan \frac{1}{57} + 28 \arctan \frac{1}{239} - 48 \arctan \frac{1}{682} + 96 \arctan \frac{1}{12943}.
\end{align*}
\]

(3.19)

The first formula was found in 1982 by K. Takano, a high school teacher and song writer. The second formula was found by F. C. W. Störmer in 1896.

Kanada and his team evaluated these formulas using a scheme analogous to that employed by Gosper and the Chudnovskys, in that they were able to avoid explicitly storing the multiprecision numbers involved. This resulted in a scheme that is roughly competitive in efficiency compared to the Salamin-Brent and Borwein quartic algorithms they had previously used, yet with a significantly lower total memory requirement. In particular, they were able to perform their latest computation on a system with 1 Thyte (10^{12} bytes) main memory, the same as with their previous computation, yet obtain six times as many digits.
After Kanada and his team verified that the hexadecimal digit strings produced by these two computations were in agreement, they performed an additional check by directly computing 20 hexadecimal digits beginning at position 1,000,000,000,001. This calculation, which employed an algorithm that we shall describe in Section 3.4 required 21 hours, much less than the time required for the first step. The result of this calculation, B4466E8D21538C4E014, perfectly agreed with the corresponding digits produced by the two arctan formulas. At this point they converted their hexadecimal value of $\pi$ to decimal, and converted back to hexadecimal as a check. These conversions employed a numerical approach similar to that used in the main and verification calculations. The entire computation, including hexadecimal and decimal evaluations and checks, required roughly 600 hours on their 64-node Hitachi parallel supercomputer. The main segment of the computation ran at nearly 1 Tflop/s (i.e., one trillion floating-point operations per second), although this performance rate was slightly lower than the rate of their previous calculation of 206 billion digits. Full details will appear in an upcoming paper [125].

According to Kanada, the ten decimal digits ending in position one trillion are 6680122702, while the ten hexadecimal digits ending in position one trillion are 3F89341CD5. Some data on the frequencies of digits in $\pi$, based on Kanada’s computations, are given in Section 4.1. Additional information of this sort is available from Kanada’s web site: http://www.supercomputing.org. Additional historical background on record-breaking computations of $\pi$ is available at http://www.cecm.sfu.ca/~jborwein/pi_cover.html. A listing of some milestones in the history of the computation of $\pi$ is given in Tables 3.1, 3.2, and 3.3.

In retrospect, one might wonder why in antiquity $\pi$ was not measured to an accuracy in excess of $\frac{22}{7}$. One conjecture is that it reflects not an inability to do so, but instead a very different mind set to a modern (Baconian) experimental one. Along this line, Marty Gerrietts, an acquaintance of one of the present authors, may provide an explanation:

I work at a youth emergency shelter and my students (right now) are 11 to 17. My youngest were as accurate as my oldest. They measured circles that I had drawn on paper . . . and used rulers to measure the string. It was probably coincidental, but they were consistently coming up with 3.1, 3.15, 3.11. That’s pretty good for string and rulers. You have to understand that they didn’t have a clue that we were finding pi. These students have very poor educational backgrounds. Those that had heard of it thought it was some magic number that only geometry teachers know about. The concept that is just a ratio between diameter and circumference had never been presented to any of them. For my convenience, I had
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<table>
<thead>
<tr>
<th>Name</th>
<th>Year</th>
<th>Digits</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Babylonians</td>
<td>2000? BCE</td>
<td>1</td>
<td>3.125 (3$\frac{1}{3}$)</td>
</tr>
<tr>
<td>Egyptians</td>
<td>2000? BCE</td>
<td>1</td>
<td>3.16045 (4(3$\frac{1}{3}$)$^2$)</td>
</tr>
<tr>
<td>China</td>
<td>1200? BCE</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Bible (1 Kings 7:23)</td>
<td>550? BCE</td>
<td>1</td>
<td>3</td>
</tr>
<tr>
<td>Archimedes</td>
<td>250? BCE</td>
<td>3</td>
<td>3.1418 (ave.)</td>
</tr>
<tr>
<td>Chang Hong</td>
<td>130 CE</td>
<td>1</td>
<td>3.1622 (\sqrt{10})</td>
</tr>
<tr>
<td>Ptolemy</td>
<td>150 CE</td>
<td>3</td>
<td>3.1466</td>
</tr>
<tr>
<td>Wang Fau</td>
<td>250 CE</td>
<td>1</td>
<td>3.15555 (\frac{142}{45})</td>
</tr>
<tr>
<td>Liu Hui</td>
<td>263 CE</td>
<td>5</td>
<td>3.14159</td>
</tr>
<tr>
<td>Siddhanta</td>
<td>380 CE</td>
<td>3</td>
<td>3.1416</td>
</tr>
<tr>
<td>Tsu Ch’ung Chi</td>
<td>480 CE</td>
<td>7</td>
<td>3.1415926 (355/113)</td>
</tr>
<tr>
<td>Aryabhata</td>
<td>499 CE</td>
<td>4</td>
<td>3.14156 (62832/2000)</td>
</tr>
<tr>
<td>Brahmagupta</td>
<td>640 CE</td>
<td>1</td>
<td>3.162277 (=\sqrt{10})</td>
</tr>
<tr>
<td>Al-Khowarizmi</td>
<td>800 CE</td>
<td>4</td>
<td>3.1416</td>
</tr>
<tr>
<td>Fibonacci</td>
<td>1220 CE</td>
<td>3</td>
<td>3.141818</td>
</tr>
<tr>
<td>Madhava</td>
<td>1400 CE</td>
<td>11</td>
<td>3.14159265359</td>
</tr>
<tr>
<td>Al-Kūshi</td>
<td>1429 CE</td>
<td>14</td>
<td>3.14159265358979</td>
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<tr>
<td>Otho</td>
<td>1573 CE</td>
<td>6</td>
<td>3.1415929</td>
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<tr>
<td>Viète</td>
<td>1593 CE</td>
<td>9</td>
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<tr>
<td>Romanus</td>
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<td>Van Ceulen</td>
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<td>Van Ceulen</td>
<td>1615 CE</td>
<td>35</td>
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Table 3.1. Pre-calculus era \(\pi\) calculations.

<table>
<thead>
<tr>
<th>Name</th>
<th>Year</th>
<th>Digits</th>
</tr>
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<tbody>
<tr>
<td>Newton</td>
<td>1665</td>
<td>16</td>
</tr>
<tr>
<td>Sharp</td>
<td>1699</td>
<td>71</td>
</tr>
<tr>
<td>Seki Kowa</td>
<td>1700</td>
<td>10</td>
</tr>
<tr>
<td>Kamata</td>
<td>1730</td>
<td>25</td>
</tr>
<tr>
<td>Machin</td>
<td>1706</td>
<td>100</td>
</tr>
<tr>
<td>De Lagny</td>
<td>1719</td>
<td>127 (112 correct)</td>
</tr>
<tr>
<td>Takebe</td>
<td>1723</td>
<td>41</td>
</tr>
<tr>
<td>Matsunaga</td>
<td>1739</td>
<td>50</td>
</tr>
<tr>
<td>Von Vega</td>
<td>1794</td>
<td>140 (136 correct)</td>
</tr>
<tr>
<td>Rutherford</td>
<td>1824</td>
<td>208 (152 correct)</td>
</tr>
<tr>
<td>Strassnitzky and Dase</td>
<td>1844</td>
<td>200</td>
</tr>
<tr>
<td>Clausen</td>
<td>1847</td>
<td>248</td>
</tr>
<tr>
<td>Lehmann</td>
<td>1853</td>
<td>261</td>
</tr>
<tr>
<td>Rutherford</td>
<td>1853</td>
<td>440</td>
</tr>
<tr>
<td>Shanks</td>
<td>1874</td>
<td>707 (527 correct)</td>
</tr>
</tbody>
</table>

Table 3.2. Calculus era \(\pi\) calculations.
<table>
<thead>
<tr>
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<th>Year</th>
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</tr>
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<tbody>
<tr>
<td>Ferguson</td>
<td>1946</td>
<td>620</td>
</tr>
<tr>
<td>Ferguson</td>
<td>1947</td>
<td>710</td>
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<tr>
<td>Ferguson and Wrench</td>
<td>1947</td>
<td>808</td>
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<tr>
<td>Smith and Wrench</td>
<td>1949</td>
<td>1,120</td>
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<tr>
<td>Reitwiesner et al. (ENIAC)</td>
<td>1949</td>
<td>2,037</td>
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<tr>
<td>Nicholson and Jeeneel</td>
<td>1954</td>
<td>3,092</td>
</tr>
<tr>
<td>Felton</td>
<td>1957</td>
<td>7,480</td>
</tr>
<tr>
<td>Genuys</td>
<td>1958</td>
<td>10,000</td>
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<tr>
<td>Felton</td>
<td>1958</td>
<td>10,021</td>
</tr>
<tr>
<td>Guilloud</td>
<td>1959</td>
<td>16,167</td>
</tr>
<tr>
<td>Shanks and Wrench</td>
<td>1961</td>
<td>100,265</td>
</tr>
<tr>
<td>Guilloud and Filliatre</td>
<td>1966</td>
<td>250,000</td>
</tr>
<tr>
<td>Guilloud and Dichampt</td>
<td>1967</td>
<td>500,000</td>
</tr>
<tr>
<td>Guilloud and Bouyer</td>
<td>1973</td>
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<tr>
<td>Miyoshi and Kanada</td>
<td>1981</td>
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<td>Guilloud</td>
<td>1982</td>
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<td>Kanada, Yoshino and Tamura</td>
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<td>Gosper</td>
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<td>Bailey</td>
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<td>Kanada and Tamura</td>
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<td>33,554,414</td>
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<tr>
<td>Kanada and Tamura</td>
<td>Jan. 1988</td>
<td>201,326,551</td>
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<tr>
<td>Chudnovskys</td>
<td>May 1989</td>
<td>480,000,000</td>
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<tr>
<td>Chudnovskys</td>
<td>Jun. 1989</td>
<td>525,229,270</td>
</tr>
<tr>
<td>Kanada and Tamura</td>
<td>Jul. 1989</td>
<td>536,870,898</td>
</tr>
<tr>
<td>Kanada and Tamura</td>
<td>Nov. 1989</td>
<td>1,073,741,799</td>
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<tr>
<td>Chudnovskys</td>
<td>Aug. 1989</td>
<td>1,011,196,691</td>
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<tr>
<td>Chudnovskys</td>
<td>Aug. 1991</td>
<td>2,260,000,000</td>
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<tr>
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<td>May 1994</td>
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<td>Takahashi and Kanada</td>
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<tr>
<td>Kanada</td>
<td>Aug. 1995</td>
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<td>Kanada</td>
<td>Oct. 1995</td>
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<td>Kanada and Takahashi</td>
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<td>51,539,600,000</td>
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<tr>
<td>Kanada and Takahashi</td>
<td>Sep. 1999</td>
<td>206,158,430,000</td>
</tr>
<tr>
<td>Kanada, Ushiro, Kuroda, Kudoh</td>
<td>Dec. 2002</td>
<td>1,241,100,000,000</td>
</tr>
</tbody>
</table>

Table 3.3. Digital era $\pi$ calculations.
made the circles with diameters of 2, 3, 4, 5 and 7. I had them measure and record the diameter, then loop the string around the circle and record the circumference. Then I had them go back and find the ratio in each case. Of course, it came to about 3 in each case and they were astounded! From there we went to a historical perspective of pi and they created their own formula for finding circumference.

In the same vein, one likely reason that Gauss and Ramanujan did not further develop the ideas in their identities for π is that an iterative algorithm, as opposed to explicit results, was not satisfactory for them (especially Ramanujan). Ramanujan would much have preferred formulae such as $\pi \approx 3 \log 5280/\sqrt{67}$ or $\pi \approx 3 \log 640320/\sqrt{163}$.

3.2 Fascination with Pi

One might wonder what has been the motivation behind these modern computations of π, given that questions such as the irrationality and transcendence of π were settled more than 100 years ago. Doubtless one motivation is simply the raw challenge of harnessing the stupendous power now available in modern computer systems for this classical computational problem. We should add that programming such calculations is definitely not trivial, especially on large, distributed memory computer systems. There have been several practical spin-off benefits from these efforts. For example, some new techniques for performing the fast Fourier transform (FFT), which is heavily used in modern science and engineering computing, had their roots in attempts to accelerate computations of π.

What’s more, it has long been recognized that the computation of π is a very strong test of computer system integrity. As we pointed out both in Section 1.3 and in our discussion above on Kanada’s calculation, such computations are typically checked by repeating the computation with a different formula, or even with a completely different computation approach. When two independent computations produce the same result, this is rather strong evidence that the computer has performed trillions of arithmetic operations, and transferred trillions of bytes of data between different components of the computer system, without error. In 1985, one of the present authors used two computations of π to test a new Cray-2 supercomputer at NASA’s Ames Research Center, and these computations in fact disclosed at least one significant hardware defect. Testing computer integrity and performance is Yasumasa Kanada’s primary motivation in the computations he has done on Hitachi supercomputers.
Beyond purely practical considerations is the continuing interest in the fundamental question of the normality (digit randomness) of $\pi$. Kanada, for example, has performed detailed statistical analysis of his computed results of $\pi$ to see if there are any statistical abnormalities that suggest $\pi$ is not normal. We shall discuss this question more fully in Section 4.1.

But there is no doubt that one motivation for computations of $\pi$ is the eternal fascination with this most prominent and mysterious of mathematical constants, a fascination shared both by professional scientists and mathematicians as well as the lay public. At the present time there are hundreds of web sites devoted to $\pi$ (see, for example, [http://www.piworld.de]), and thousands of online research papers and other documents dealing with $\pi$. There are even several Internet-based clubs devoted to $\pi$, one of which requires that initiates recite by heart the first 100 digits of $\pi$ with “respect, fluency, and smoothness” (see [http://pi314.at]). The very popular web-site [http://www.cecm.sfu.ca/pi/yapPing.html] recites $\pi$ in many different languages.

Fascination with $\pi$ is also evident in the many recent popular books, television shows, and movies that have mentioned $\pi$. In the 1967 Star Trek episode “Wolf in the Fold,” Spock foiled the evil computer by telling it to compute the last digit of $\pi$. A May 1993 segment of The Simpsons featured the character Apu boasting that he can recite $\pi$ to 40,000 digits, and that the last digit is a “1” (one of the present authors was asked by the show’s writers for this digit) [157]. In November 1996, the MSNBC network aired a news segment about $\pi$, including interviews with one of the present authors and several other mathematicians at Simon Fraser University. The 1997 movie Contact, starring Jodie Foster, was based on the 1986 book by noted astronomer Carl Sagan. In the book version, the lead female character searched for patterns in the digits of $\pi$, and after her mysterious experience found confirmation in the base-11 expansion of $\pi$ [177]. A 1997 book entitled The Joy of Pi sold thousands of copies [38]. A 1998 movie entitled Pi began with decimal digits of $\pi$ displayed on the screen. The 2001 Academy Award-winning movie A Beautiful Mind, which portrayed the life of mathematician John Nash, shows $\pi$ in equations scribbled by the lead actor Russell Crowe (although the $\pi$ characters here appear to denote the prime-counting function and other nongeometric entities). The 2002 book Life of Pi by Canadian author Yann Martel won the Booker Prize, a prestigious British literary award [152]. Finally, in the 2003 movie Matrix Reloaded, the Key Maker warns that a door will be accessible for exactly 314 seconds, a figure that Time speculated was a reference to $\pi$ [76].

Along this line, National Public Radio reported on April 12, 2003 that novelty automatic teller machine withdrawal slips, showing a balance of $314,159.26, are popular in New York City. One can scribble a note on
the back and, apparently innocently, let the intended target be suitably impressed by one’s amazingly healthy saving account. Scott Simon, the host of this NPR show, noted the close resemblance to $\pi$.

For those who know *The Hitchhiker’s Guide to the Galaxy*, it is amusing that 042 occurs at the digits ending at the fifty-billionth decimal place in each of $\pi$ and $1/\pi$—thereby providing an excellent answer to the ultimate question, “What is forty two?”

It is hard to imagine $e$ or $\log 2$ playing the same role. That said, the publicity surrounding the Millennium problems has lead to a spate of recent popular books on the Riemann Hypothesis. The million dollar prize for the Riemann Hypothesis even formed the basis of a recent episode of the television program *Law and Order*, in which student notebooks contained quite accurate formulas.

### 3.3 Behind the Cubic and Quartic Iterations

The genesis of the $\pi$ algorithms (3.13), (3.17), (3.18) and related material is itself an illustrative example of experimental mathematics. For nonnegative integer $N$, the function

$$
\alpha(N) = \frac{E'(k_N)}{K(k_N)} - \frac{\pi}{4K^2(k_N)}
$$

had arisen, where $k_N$ is the $N$-th singular value, and $K$ and $E'$ are complete elliptic integrals as detailed in the discussion of Legendre’s relation in Section 5.6.1. For present purposes, it suffices that (3.20) is very easy to compute. For example, the first few non-composite values are (to 20 digit accuracy):

- $\alpha(1) \approx 0.49999999999999999999$
- $\alpha(2) \approx 0.41421356237309504880$
- $\alpha(3) \approx 0.36602540378443864678$
- $\alpha(5) \approx 0.33188261099247156221$
- $\alpha(7) \approx 0.32287565553229529536$

It is obvious that $\alpha(1) = 1/2$ and easy to spot that $\alpha(2) = \sqrt{2} - 1$, from which it was quickly observed that $\alpha(3) = (\sqrt{3} - 1)/2$ and that $\alpha(7) = (\sqrt{7} - 2)/2$, but $\alpha(5)$ did not appear to be a quadratic. Twenty years ago, such identification was not as easy, and it was only when it occurred to the Borweins that quadratic fields congruent to $\pm 1 \mod 4$ behave differently that they stumbled upon (experimentally) the identity

$$
\alpha(5) = \frac{\sqrt{5} - \sqrt{2} \sqrt{5} - 2}{2}.
$$

(3.21)
Nowadays, this is almost trivial: A “Minpoly” calculation immediately returns $29 - 80x - 24x^2 + 16x^4 = 0$ and this has the surd above as its smallest positive root. At this point, the authors could use known results only to prove the value of $\alpha(1), \alpha(2)$ and $\alpha(3)$. Those for $\alpha(5)$ and $\alpha(7)$ remained conjectural. There was, however, an empirical family of algorithms for $\pi$: let $\alpha_0 = \alpha(N)$ and $k_0 = k'_N$ (where $k' = \sqrt{1 - k^2}$) and iterate

$$k_{n+1} = \frac{1 - k'_n}{1 + k'_n} \quad \text{(3.22)}$$

$$\alpha_{n+1} = (1 + k_{n+1})^2 \alpha_n - \sqrt{N} 2^{n+1} k_{n+1}. \quad \text{(3.23)}$$

Then

$$\lim_{n \to \infty} \alpha_n^{-1} = \pi. \quad \text{(3.24)}$$

Again, (3.24) was provable for $N = 1, 2, 3$ and only conjectured for $N = 5, 7$. In each case the algorithm appeared to converge quadratically to $\pi$. On closer inspection while the provable cases were correct to 5,000 digits, the empirical ones agreed with $\pi$ to roughly 100 places only. Now, in many ways to have discovered a “natural” number that agreed with $\pi$ to that level—and no more—would have been more interesting than the alternative. That seemed unlikely, but recoding and rerunning the iterations kept producing identical results.

Twenty years ago, very high-precision calculation was less accessible, and the code was being run in a Berkeley Unix integer package. After about six weeks of effort, it was found that the square root algorithm in the package was badly flawed, but only if run with an odd precision of more than 60 digits! And for idiosyncratic reasons that had only been the case in the two unproven cases. Needless to say, tracing the bug was a salutary and somewhat chastening experience.

### 3.4 Computing Individual Digits of Pi

An outsider might be forgiven for thinking that essentially everything of interest with regards to $\pi$ has been discovered. For example, this sentiment is suggested in the closing chapters of Beckmann’s 1971 book on the history of $\pi$ [33, pg. 172]. Ironically, the Salamin–Brent quadratically convergent iteration was discovered only five years later, and the higher-order convergent algorithms followed in the 1980s. In 1990, Rabinowitz and Wagon discovered a “spigot” algorithm for $\pi$, which permits successive digits of $\pi$ (in any desired base) to be computed with a relatively simple recursive
3.4. Computing Individual Digits of Pi

algorithm based on the previously generated digits (see [169] and Item [15] at the end of this chapter).

But even insiders are sometimes surprised by a new discovery. Prior to 1996, almost all mathematicians believed that if you want to determine the $d$-th digit of $\pi$, you have to generate the entire sequence of the first $d$ digits. (For all of their sophistication and efficiency, the schemes described above all have this property.) But it turns out that this is not true, at least for hexadecimal (base 16) or binary (base 2) digits of $\pi$. In 1996, Peter Borwein, Simon Plouffe, and one of the present authors (Bailey) found an algorithm for computing individual hexadecimal or binary digits of $\pi$ [21].

To be precise, this algorithm:

(1) directly produces a modest-length string of digits in the hexadecimal or binary expansion of $\pi$, beginning at an arbitrary position, without needing to compute any of the previous digits;

(2) can be implemented easily on any modern computer;

(3) does not require multiple precision arithmetic software;

(4) requires very little memory; and

(5) has a computational cost that grows only slightly faster than the digit position.

Using this algorithm, for example, the one millionth hexadecimal digit (or the four millionth binary digit) of $\pi$ can be computed in less than a minute on a 2003-era computer. The new algorithm is not fundamentally faster than best-known schemes for computing all digits of $\pi$ up to some position, but its elegance and simplicity are nonetheless of considerable interest. This scheme is based on the following remarkable new formula for $\pi$:

**Theorem 3.2.**

$$\pi = \sum_{i=0}^{\infty} \frac{1}{16^i} \left( \frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6} \right). \quad (3.25)$$

**Proof.** First note that for any $k < 8$,

$$\int_0^{1/\sqrt{2}} \frac{x^{k-1}}{1-x^8} \, dx = \int_0^{1/\sqrt{2}} \sum_{i=0}^{\infty} x^{k-1+8i} \, dx$$

$$= \frac{1}{2^{k/2}} \sum_{i=0}^{\infty} \frac{1}{16^i (8i+k)} \quad (3.26)$$
Thus one can write
\[
\sum_{i=0}^{\infty} \frac{1}{16^i} \left( \frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6} \right)
\]
\[
= \int_{0}^{1/\sqrt{2}} \frac{4\sqrt{2} - 8x^3 - 4\sqrt{2}x^4 - 8x^5}{1 - x^5} \, dx,
\] (3.27)
which on substituting \( y = \sqrt{2}x \) becomes
\[
\int_{0}^{1} \frac{16y - 16}{y^4 - 2y^3 + 4y - 4} \, dy = \int_{0}^{1} \frac{4y}{y^2 - 2} \, dy - \int_{0}^{1} \frac{4y - 8}{y^2 - 2y + 2} \, dy
\]
\[
= \pi. \tag{3.28}
\]

However, in presenting this formal derivation, we are disguising the actual route taken to the discovery of this formula. This route is a superb example of experimental mathematics in action.

It all began in 1995, when Peter Borwein and Simon Plouffe of Simon Fraser University observed that the following well-known formula for \( \log 2 \) permits one to calculate isolated digits in the binary expansion of \( \log 2 \):
\[
\log 2 = \sum_{k=0}^{\infty} \frac{1}{k2^k}. \tag{3.29}
\]
This scheme is as follows. Suppose we wish to compute a few binary digits beginning at position \( d + 1 \) for some integer \( d > 0 \). This is equivalent to calculating \( \{2^d \log 2\} \), where \( \{ \cdot \} \) denotes fractional part. Thus we can write
\[
\{2^d \log 2\} = \left\{ \left\{ \sum_{k=0}^{d} \frac{2^{d-k}}{k} \right\} + \sum_{k=d+1}^{\infty} \frac{2^{d-k}}{k} \right\}
\]
\[
= \left\{ \sum_{k=0}^{d} \frac{2^{d-k} \mod k}{k} \right\} + \sum_{k=d+1}^{\infty} \frac{2^{d-k}}{k}. \tag{3.30}
\]
We are justified in inserting “\( \mod k \)” in the numerator of the first summation, because we are only interested in the fractional part of the quotient when divided by \( k \).

Now the key observation is this: The numerator of the first sum in Equation (3.30), namely \( 2^{d-k} \mod k \), can be calculated very rapidly by
means of the binary algorithm for exponentiation, performed modulo \( k \). The binary algorithm for exponentiation is merely the formal name for the observation that exponentiation can be economically performed by means of a factorization based on the binary expansion of the exponent. For example, we can write \( 3^{17} = (((3^2)^2)^2)^2 \cdot 3 \), thus producing the result in only 5 multiplications, instead of the usual 16. According to Knuth, this technique dates back at least to 200 BCE \[130\] pg. 461. In our application, we need to obtain the exponentiation result modulo a positive integer \( k \). This can be done very efficiently by reducing modulo \( k \) the intermediate multiplication result at each step of the binary algorithm for exponentiation. A formal statement of this scheme is as follows:

**Algorithm 3.3. Binary algorithm for exponentiation modulo \( k \).**

To compute \( r = b^n \mod k \), where \( r, b, n \) and \( k \) are positive integers: First set \( t \) to be the largest power of two such that \( t \leq n \), and set \( r = 1 \). Then

\[
A: \text{if } n \geq t \text{ then } r \leftarrow br \mod k; \quad n \leftarrow n - t; \quad \text{endif}
\]

\[
t \leftarrow t/2
\]

if \( t \geq 1 \) then \( r \leftarrow r^2 \mod k \); go to A; endif

Note that the above algorithm is performed entirely with positive integers that do not exceed \( k^2 \) in size. Thus ordinary 64-bit floating-point or integer arithmetic, available on almost all modern computers, suffices for even rather large calculations. 128-bit floating-point arithmetic (double-double or quad precision), available at least in software on many systems (see Section 6.2.1), suffices for the largest computations currently feasible.

We can now present the algorithm for computing individual binary digits of \( \log 2 \).

**Algorithm 3.4. Individual digit algorithm for \( \log 2 \).**

To compute the \((d + 1)\)-th binary digit of \( \log 2 \): Given an integer \( d > 0 \), (1) calculate each numerator of the first sum in Equation (3.30), using Algorithm 3.0, implemented using ordinary 64-bit or 128-bit floating-point arithmetic; (2) divide each numerator by the respective value of \( k \), again using ordinary floating-point arithmetic; (3) sum the terms of the first summation, while discarding any integer parts; (4) evaluate the second summation as written using floating-point arithmetic—only a few terms are necessary since it rapidly converges; and (5) add the result of the first and second summations, discarding any integer part. The resulting fraction, when expressed in binary, gives the first few digits of the binary expansion of \( \log 2 \) beginning at position \( d + 1 \). \( \square \)
As soon as Borwein and Plouffe found this algorithm, they began seeking other mathematical constants that shared this property. It was clear that any constant \( \alpha \) of the form

\[
\alpha = \sum_{k=0}^{\infty} \frac{p(k)}{q(k)2^k},
\]

Equation (3.31)

where \( p(k) \) and \( q(k) \) are integer polynomials, with \( \text{deg} \, p < \text{deg} \, q \) and \( q \) having no zeroes at nonnegative integer arguments, is in this class. Further, any rational linear combination of such constants also shares this property. Checks of various mathematical references eventually uncovered about 25 constants that possessed series expansions of the form given by Equation (3.31).

As you might suppose, the question of whether \( \pi \) also shares this property did not escape these researchers. Unfortunately, exhaustive searches of the mathematical literature did not uncover any formula for \( \pi \) of the requisite form. But given the fact that any rational linear combination of constants with this property also shares this property, Borwein and Plouffe performed integer relation searches to see if a formula of this type existed for \( \pi \). This was done, using computer programs written by one of the present authors (Bailey), which implement the “PSLQ” integer relation algorithm in high-precision, floating-point arithmetic [92, 13]. We will discuss the PSLQ algorithm and related techniques more in Section 6.3.

In particular, these three researchers sought an integer relation for the real vector \((\alpha_1, \alpha_2, \cdots, \alpha_n)\), where \( \alpha_1 = \pi \) and \((\alpha_i, \, 2 \leq i \leq n)\) is the collection of constants of the requisite form gleaned from the literature, each computed to several hundred decimal digit precision. To be precise, they sought an \( n \)-long vector of integers \((a_i)\) such that

\[
\sum a_i \alpha_i = 0,
\]

within a very small “epsilon.” After a month or two of computation, with numerous restarts using new \( \alpha \) vectors (when additional formulas were found in the literature) the identity (3.25) was finally uncovered. The actual formula found by the computation was:

\[
\pi = 4F(1, 1/4; 5/4; -1/4) + 2 \arctan(1/2) - \log 5,
\]

Equation (3.32)

where \( F(1, 1/4; 5/4; -1/4) = 0.955933837\ldots \) is a hypergeometric function evaluation. Reducing this expression to summation form yields the new \( \pi \) formula:

\[
\pi = \sum_{i=0}^{\infty} \frac{1}{16^i} \left( \frac{4}{8i-1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6} \right).
\]

Equation (3.33)

To return briefly to the derivation of Formula (3.33), let us point out that it was discovered not by formal reasoning, or even by computer-based
symbolic processing, but instead by numerical computations using a high-precision implementation of the PSLQ integer relation algorithm. It is most likely the first instance in history of the discovery of a new formula for π by a computer. We might mention that, in retrospect, Formula (3.33) could be found much more quickly, by seeking integer relations in the vector \((\pi, S_1, S_2, \cdots, S_8)\), where

\[
S_j = \sum_{k=0}^{\infty} \frac{1}{16^k(8k + j)}.
\] (3.34)

Such a calculation could be done in a few seconds on a computer, even if one did not know in advance to use 16 in the denominator and 9 terms in the search, but instead had to stumble on these parameters by trial and error. But this observation is, as they say, 20-20 hindsight. The process of real mathematical discovery is often far more tortuous and less elegant than the polished version typically presented in textbooks and research journals.

It should be clear at this point that the scheme for computing individual hexadecimal digits of π is very similar to Algorithm 3.0. For completeness, we state it as follows:

**Algorithm 3.5. Individual digit algorithm for π.**

To compute the \((d + 1)\)-th hexadecimal digit of π: Given an integer \(d > 0\), we can write

\[
\{16^d\pi\} = \{4\{16^dS_1\} - 2\{16^dS_4\} - \{16^dS_5\} - \{16^dS_6\}\}, \tag{3.35}
\]

using the \(S_j\) notation of Equation (3.34). Now apply Algorithm 3.0 with

\[
\{16^dS_j\} = \left\{ \left\{ \sum_{k=0}^{d} \frac{16^{d-k}}{8k + j} \right\} + \sum_{k=d+1}^{\infty} \frac{16^{d-k}}{8k + j} \right\}
\]

\[
= \left\{ \left\{ \sum_{k=0}^{d} \frac{16^{d-k} \mod 8k + j}{8k + j} \right\} + \sum_{k=d+1}^{\infty} \frac{16^{d-k}}{8k + j} \right\} \tag{3.36}
\]

instead of Equation (3.30), to compute \(\{16^dS_j\}\) for \(j = 1, 4, 5, 6\). Combine these four results, discarding integer parts, as shown in (3.35). The resulting fraction, when expressed in hexadecimal notation, gives the hex digit of π in position \(d + 1\), plus a few more correct digits.

As with Algorithm 3.0, multiple-precision arithmetic software is not required—ordinary 64-bit or 128-bit floating-point arithmetic suffices even
for some rather large computations. We have omitted here some numerical
details for large computations—see [21]. Sample implementations in both C
and Fortran-90 are available from the web site [http://www.experimentalmath.info].

One mystery that remains unanswered is why Formula (3.33) was not
discovered long ago. As you can see from the above proof, there is nothing
very sophisticated about its derivation. There is no fundamental reason
why Euler, for example, or Gauss or Ramanujan, could not have discov-
ered it. Perhaps the answer is that its discovery was a case of “reverse
mathematical engineering.” Lacking a motivation to find such a formula,
mathematicians of previous eras had no reason to derive one. But this still
doesn’t answer the question of why the algorithm for computing individual
digits of log 2 had not been discovered before—it is based on a formula,
namely Equation (3.29), that has been known for centuries.

Needless to say, Algorithm 3.0 has been implemented by numerous re-
searchers. In 1997, Fabrice Bellard of INRIA computed 152 binary digits of
π starting at the trillionth binary digit position. The computation took 12
days on 20 workstations working in parallel over the Internet. His scheme
is actually based on the following variant of 3.33:

\[
\pi = 4 \sum_{k=0}^{\infty} \frac{(-1)^k}{4^k(2k + 1)} - \frac{1}{64} \sum_{k=0}^{\infty} \frac{(-1)^k}{1024^k} \left( \frac{32}{4k+1} + \frac{8}{4k+2} + \frac{1}{4k+3} \right). \quad (3.37)
\]

This formula permits individual hex or binary digits of π to be calculated
roughly 43% faster than (3.25).

A year later, Colin Percival, then a 17-year-old student at Simon Fraser
University, utilized a network of 25 machines to calculate binary digits in
the neighborhood of position 5 trillion, and then in the neighborhood of 40
trillion. In September 2000, he found that the quadrillionth binary digit
is “0,” based on a computation that required 250 CPU-years of run time,
carried out using 1,734 machines in 56 countries. Table 3.4 gives some
results known as of this writing.

One question that immediately arises in the wake of this discovery is
whether or not there is a formula of this type and an associated compu-
tational scheme to compute individual decimal digits of π. Searches con-
ducted by numerous researchers have been unfruitful. Now it appears that
there is no nonbinary formula of this type—this is ruled out by a new result
co-authored by one of the present authors (see Section 3.7) [48]. However,
none of this removes the possibility that there exists some completely differ-
ent approach that permits rapid computation of individual decimal digits
3.5. Unpacking the BBP Formula for Pi

It is worth asking “why” the formula

\[ \pi = \sum_{i=0}^{\infty} \frac{1}{16^i} \left( \frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6} \right) \]  \hspace{1cm} (3.38)  

exists. As observed above, this identity is equivalent to, and can be proved by establishing:

\[ \pi = \int_{0}^{1/\sqrt{2}} \frac{4\sqrt{2} - 8x^3 - 4\sqrt{2}x^4 - 8x^5}{1 - x^8} \, dx. \]

The present version of Maple evaluates this integral to

\[ -2 \log 2 + 2 \log(2 - \sqrt{2}) + \pi + 2 \log(2 + \sqrt{2}), \]  \hspace{1cm} (3.39)

which simplifies to \( \pi \). In any event, one can ask what the individual series in (3.38) comprise. So consider

\[ S_b = \sum_{k=0}^{\infty} \frac{1}{16^k(8k+b)} \]
for $1 \leq b \leq 8$ and the corresponding normalized integrals

$$I(b) = 2^{b/2} \int_{0}^{1} \frac{x^{b-1}}{1-x^b} \, dx. \quad (3.40)$$

Again, Maple provides closed forms for $I(b)$ in which the basic quantities seem to be the following: $\arctan(2)$, $\arctan(1/2)$, $\sqrt{2} \arctan(1/\sqrt{2})$, $\log(2)$, $\log(3)$, $\log(5)$, and $\log(\sqrt{2} \pm 1)$. At this point one may use integer relation methods and obtain:

$$S_1 = \frac{\pi}{8} + \frac{\log 5}{8} - \frac{\sqrt{2} \log(\sqrt{2} - 1)}{4} - \frac{\arctan(1/2)}{4} + \frac{\sqrt{2} \arctan(\sqrt{2}/2)}{4}$$

$$S_2 = \frac{\log(3)}{4} + \frac{\arctan(1/2)}{2}$$

$$S_3 = \frac{\pi}{4} - \frac{\sqrt{2} \log(\sqrt{2} - 1)}{2} - \frac{\arctan(1/2)}{2} - \frac{\sqrt{2} \arctan(\sqrt{2}/2)}{2} - \frac{\log 5}{4}$$

$$S_4 = \frac{\log 5}{2} - \frac{\log 3}{2}$$

$$S_5 = -\frac{\pi}{2} - \frac{\sqrt{2} \log(\sqrt{2} - 1)}{2} + \frac{\arctan(1/2)}{2} + \frac{\sqrt{2} \arctan(\sqrt{2}/2)}{2} - \frac{\log 5}{2}$$

$$S_6 = \log(3) - 2 \arctan(1/2)$$

$$S_7 = -\pi + \log 5 - 2\sqrt{2} \log(\sqrt{2} - 1) + 2 \arctan(1/2) - 2\sqrt{2} \arctan(\sqrt{2}/2)$$

$$S_8 = 8 \log 2 - 2 \log 5 - 2 \log 3. \quad (3.41)$$

Thus the “simple” hexadecimal formula (3.38) is actually a molecule made up of more subtle hexadecimal atoms: with the final bond coming from the simple identity $\arctan 2 + \arctan(1/2) = \pi/2$. As an immediate consequence, one obtains the formula $\arctan(1/2) = S_2 - S_6/4$.

Furthermore, the facts that

$$\text{Im} \left( \log \left( \frac{1}{1 - \frac{1}{x}} \right) \right) = \arctan \left( \frac{1}{1-x} \right)$$

$$2 \arctan(1/3) + \arctan(1/7) = \arctan(1/2) + \arctan(1/3)$$

$$= \arctan 1 = \pi/4 \quad (3.42)$$

allow one to write directly a base-64 series for $\arctan(1/3)$ (using $x = 4$) and a base-1024 series for $\arctan(1/7)$ (using $x = 8$). This yields the identity

$$\frac{\pi}{4} = \frac{1}{16} \sum_{n=0}^{\infty} \frac{(-1)^n}{64^n} \left( \frac{8}{4n + 1} + \frac{4}{4n + 2} + \frac{1}{4n + 3} \right)$$

$$+ \frac{1}{256} \sum_{n=0}^{\infty} \frac{(-1)^n}{1024^n} \left( \frac{32}{4n + 1} + \frac{8}{4n + 2} + \frac{1}{4n + 3} \right), \quad (3.43)$$
which is similar to, although distinct from, the identity used by Bellard
and Percival in their computations.

3.6 Other BBP-Type Formulas

A formula of the type mentioned in the previous sections, namely

\[ \alpha = \sum_{k=0}^{\infty} \frac{p(k)}{b^k q(k)}, \quad (3.44) \]

is now referred to as a BBP-type formula, named after the initials of the
authors of the 1997 paper where the \( \pi \) hex digit algorithm appeared \[21\].
For a constant \( \alpha \) given by a formula of this type, it is clear that individual
base-\( b \) digits can be calculated, using the scheme similar to the ones outlined
in the previous section. The paper \[21\] includes formulas of this type for
several other constants. Since then, a large number of other BBP-type
formulas have been discovered.

Most of these identities were discovered using an experimental ap-
proach, using PSLQ searches. Others were found as the result of educated
guesses based on experimentally obtained results. In each case, these for-
mulas have been formally established, although the proofs are not always
as simple as the proof of Theorem 3.0 We present these results, in part,
to underscore the fact that the approach used to find the new formula for
\( \pi \) has very broad applicability.

A sampling of the known binary BBP-type formulas (i.e., formulas with
a base \( b = 2^p \) for some integer \( p \)) is shown in Table 3.6. Some nonbinary
BBP-type formulas are shown in Table 3.7. These formulas are derived
from several sources: \[21\] \[60\] \[61\]. An updated collection is available at
[16]. The constant \( G \) that appears in Table 3.6 is Catalan’s constant,
namely \( G = 1 - 1/3^2 + 1/5^2 - 1/7^2 + \cdots = 0.9159655941\ldots \)

In addition to the formulas in Tables 3.6 and 3.7, there are two other
classes of constants known to possess binary BBP-type formulas. The
first is logarithms of certain integers. Clearly, \( \log n \) can be written with
a binary BBP formula (i.e. a formula with \( b = 2^m \) for some integer \( m \))
provided \( n \) factors completely using primes whose logarithms have binary
BBP formulas—one merely combines the individual series for the different
primes into a single binary BBP formula. We have seen that the logarithm
of the prime 2 possesses a binary BBP formula, and so does \( \log 3 \), by the
following reasoning:

\[
\log 3 = 2 \log 2 + \log \left(1 - \frac{1}{4}\right) = 2 \sum_{k=1}^{\infty} \frac{1}{k2^k} - \sum_{k=1}^{\infty} \frac{1}{k4^k}
\]

\[
= \frac{1}{2} \sum_{k=0}^{\infty} \frac{1}{4^k} \left(\frac{2}{2k+1} + \frac{1}{2k+2}\right) - \frac{1}{4} \sum_{k=0}^{\infty} \frac{1}{4^k} \left(\frac{2}{2k+2}\right)
\]

\[
= \sum_{k=0}^{\infty} \frac{1}{4^k} \left(\frac{1}{2k+1}\right). \quad (3.45)
\]

In a similar manner, it can be shown, by examining the factorization of \(2^n + 1\) and \(2^n - 1\), where \(n\) is an integer, that numerous other primes have this property. Some additional primes can be obtained by noting that the real part of the Taylor series expansion of

\[
\alpha = \log \left(1 \pm \frac{(1+i)^k}{2^n}\right) \quad (3.46)
\]

yields a BBP-type formula. See [16] for details.

The logarithms of the following primes are now known to possess binary BBP formulas [68]:

\[
\begin{align*}
2, & \quad 3, & \quad 5, & \quad 7, & \quad 11, & \quad 13, & \quad 17, & \quad 19, & \quad 29, & \quad 31, & \quad 37, & \quad 41, & \quad 43, & \quad 61, & \quad 73, & \quad 109, & \quad 113, & \quad 127, & \quad 151, & \quad 241, & \quad 257, & \quad 331, & \quad 337, & \quad 397, & \quad 683, & \quad 1321, & \quad 1429, & \quad 1613, & \quad 2113, & \quad 2731, & \quad 5419, & \quad 8191, & \quad 14449, & \quad 26317, & \quad 38737, & \quad 43691, & \quad 65537, & \quad 87211, & \quad 131071, & \quad 174763, & \quad 246241, & \quad 262657, & \quad 268501, & \quad 279073, & \quad 312709, & \quad 524287, & \quad 525313, & \quad 599479, & \quad 2796203, & \quad 4327489, & \quad 7416361, & \quad 15790321, & \quad 18837001, & \quad 22366891
\end{align*}
\]

This list is certainly not complete, and it is unknown whether or not all primes have this property, or even whether the list of such primes is finite or infinite. One can also obtain BBP-type formulas in nonbinary bases for the logarithms of certain integers and rational numbers. One example is given by the base ten formula for \(\log(9/10)\) in Table 3.7. This has been used to compute the ten billionth decimal digit of \(\log(9/10)\) [21].

One additional class of binary BBP-type formulas that we will mention here is arctangents of certain rational numbers. We present here the results of experimental searches, using the PSLQ integer relation algorithm, which we have subsequently established formally. The formal derivation of these results proceeds as follows. Consider the set of rationals given by

\[
q = \left|\frac{\text{Im}(T)}{\text{Re}(T)}\right| \quad \text{or} \quad \left|\frac{\text{Re}(T)}{\text{Im}(T)}\right|,
\]

where

\[
T = \prod_{k=1}^{m} \left(1 \pm \frac{i}{2^{v_k}}\right)^{u_k} \left(1 \pm \frac{1 + i}{2^{v_k}}\right)^{w_k} \quad (3.48)
\]
3.6. Other BBP-Type Formulas

for various \( m \)-long nonnegative integer vectors \( t, u, v, w \) and choices of signs as shown [49, pg. 344]. For example, setting \( t = (1, 1), u = (1, 1), v = (1, 3), w = (1, 1), \) with signs \((1, -1, -1, 1)\), gives the result \( T = \frac{25}{32} - \frac{5i}{8} \), which yields \( q = \frac{4}{5} \). Indeed, one can obtain the formula

\[
\arctan \left( \frac{4}{5} \right) = \frac{1}{2^{17}} \sum_{k=0}^{\infty} \frac{1}{2^{20k}} \left( \frac{524288}{40k + 2} - \frac{393216}{40k + 4} - \frac{491520}{40k + 5} + \frac{163840}{40k + 8} + \frac{32768}{40k + 10} - \frac{24576}{40k + 12} + \frac{5120}{40k + 15} + \frac{10240}{40k + 16} + \frac{2048}{40k + 18} + \frac{1024}{40k + 20} + \frac{640}{40k + 24} + \frac{480}{40k + 25} + \frac{128}{40k + 26} - \frac{96}{40k + 28} + \frac{40}{40k + 32} + \frac{8}{40k + 34} \right) \left( \frac{5}{40k + 35} - \frac{6}{40k + 36} \right). \tag{3.49} \]

The set of rationals for which BBP formulas can be obtained in this way can be further expanded by applying the formula

\[
\tan(r + s) = \frac{\tan r + \tan s}{1 - \tan(r)s}, \tag{3.50} \]

for rationals \( r \) and \( s \) for which binary BBP-type formulas are found. By applying these methods, it can be shown that binary BBP formulas exist for the arctangents of the rationals shown in Table 3.5, where only those rationals with numerators \(<\) denominators \(\leq 25\) are listed. Note that not all “small” rationals appear in this list. As it turns out, by applying the methods given in the paper [48] (see the next section), one can rule out the possibility of Machin-type BBP formulas (as described in Section 3.6) for the arctangents of \(2/7, 3/8, 5/8, 4/9, \) and \(5/9\). Thus we believe the above list to be complete for rationals with numerators and denominators up to ten. Beyond this level, we do not know for sure whether this list is complete, or whether applying formula (3.48), together with addition and subtraction formulas, generates all possible rationals possessing binary BBP-type formulas.

One can obtain BBP formulas in nonbinary bases for the arctangents of certain rational numbers by employing an appropriate variant of formula (3.48).
3.7 Does Pi Have a Nonbinary BBP Formula?

As we mentioned above, from the day that the BBP-formula for $\pi$ was discovered, many researchers have wondered whether there exist BBP-type formulas that would permit computation of individual digits in bases other than powers of two (such as base ten). This is not such a far-fetched possibility, because both base-2 and base-3 formulas are known for $\pi^2$, as well as for $\log 2$ (see Tables 3.6 and 3.7). But extensive computations failed to find any nonbinary formulas for $\pi$.

Recently one of the present authors, together with David Borwein (Jon’s father) and William Galway, established that there are no nonbinary Machin-type arctangent formulas for $\pi$. We believe that if there is no nonbinary Machin-type arctangent formula for $\pi$, then there is no nonbinary BBP-type formula of any form for $\pi$. We will summarize this result here. Full details and other related results can be found in [48].

We say that the integer $b > 1$ is not a proper power if it cannot be written as $c^n$ for any integers $c$ and $m > 1$. We will use the notation $\text{ord}_p(z)$ to denote the $p$-adic order of the rational $z \in Q$. In particular, $\text{ord}_p(p) = 1$ for prime $p$, while $\text{ord}_p(q) = 0$ for primes $q \neq p$, and $\text{ord}_p(wz) = \text{ord}_p(w) + \text{ord}_p(z)$. The notation $\nu_0(p)$ will mean the order of the integer $b$ in the multiplicative group of the integers modulo $p$. We will say that $p$ is a primitive prime factor of $b^m - 1$ if $m$ is the least integer such that $p| (b^m - 1)$. Thus $p$ is a primitive prime factor of $b^m - 1$ provided $\nu_0(p) = m$.

Given the Gaussian integer $z \in Q[i]$ and the rational prime $p \equiv 1$ (mod 4), let $\theta_p(z)$ denote $\text{ord}_p(z) - \text{ord}_p(\bar{z})$, where $p$ and $\bar{p}$ are the two conjugate
3.7. Does Pi Have a Nonbinary BBP Formula?

\[
\begin{align*}
\pi \sqrt{3} &= \frac{9}{32} \sum_{k=0}^{\infty} \frac{1}{64^k} \left( \frac{16}{6k+1} + \frac{8}{6k+2} - \frac{2}{6k+4} - \frac{1}{6k+5} \right) \\
\pi^2 &= \frac{9}{8} \sum_{k=0}^{\infty} \frac{1}{64^k} \left( \frac{16}{(6k+1)^2} - \frac{24}{(6k+2)^2} - \frac{8}{(6k+3)^2} - \frac{6}{(6k+4)^2} \right) \\
&\quad + \frac{1}{(6k+5)^2} \\
\log^2 2 &= \frac{1}{32} \sum_{k=0}^{\infty} \frac{1}{64^k} \left( \frac{64}{(6k+1)^2} - \frac{160}{(6k+2)^2} - \frac{56}{(6k+3)^2} - \frac{40}{(6k+4)^2} \right) \\
&\quad + \frac{4}{(6k+5)^2} - \frac{1}{(6k+6)^2} \\
\pi \log 2 &= \frac{1}{256} \sum_{k=0}^{\infty} \frac{1}{4096^k} \left( \frac{4096}{(24k+1)^2} - \frac{8192}{(24k+2)^2} - \frac{26112}{(24k+3)^2} \right) \\
&\quad + \frac{15360}{(24k+4)^2} - \frac{1024}{(24k+5)^2} + \frac{9984}{(24k+6)^2} + \frac{11520}{(24k+8)^2} \\
&\quad + \frac{2368}{(24k+9)^2} - \frac{512}{(24k+10)^2} + \frac{768}{(24k+12)^2} - \frac{64}{(24k+13)^2} \\
&\quad + \frac{488}{(24k+15)^2} + \frac{720}{(24k+16)^2} + \frac{16}{(24k+17)^2} + \frac{196}{(24k+18)^2} \\
&\quad + \frac{60}{(24k+20)^2} - \frac{37}{(24k+21)^2} \\
G &= \frac{1}{1024} \sum_{k=0}^{\infty} \frac{1}{4096^k} \left( \frac{3072}{(24k+1)^2} - \frac{3072}{(24k+2)^2} - \frac{23040}{(24k+3)^2} \right) \\
&\quad + \frac{12288}{(24k+4)^2} - \frac{768}{(24k+5)^2} + \frac{9216}{(24k+6)^2} + \frac{10368}{(24k+8)^2} \\
&\quad + \frac{2496}{(24k+9)^2} - \frac{192}{(24k+10)^2} + \frac{768}{(24k+12)^2} - \frac{48}{(24k+13)^2} \\
&\quad + \frac{360}{(24k+15)^2} + \frac{648}{(24k+16)^2} + \frac{12}{(24k+17)^2} + \frac{168}{(24k+18)^2} \\
&\quad + \frac{48}{(24k+20)^2} - \frac{39}{(24k+21)^2}
\end{align*}
\]

Table 3.6. Binary BBP-type formulas.
\[
\log 2 = \frac{2}{3} \sum_{k=0}^{\infty} 9^k (2k + 1)
\]
\[
\pi \sqrt{3} = \frac{1}{9} \sum_{k=0}^{\infty} \frac{729^k}{12k+1} \left( \frac{81}{12k+2} - \frac{54}{12k+3} - \frac{9}{12k+4} - \frac{12}{12k+6} \right)
\]
\[
\log 3 = \frac{1}{729} \sum_{k=0}^{\infty} \frac{1}{729^k} \left( \frac{729}{6k+1} + \frac{81}{6k+2} + \frac{81}{6k+3} + \frac{9}{6k+4} \right)
\]
\[
\pi^2 = \frac{2}{27} \sum_{k=0}^{\infty} \frac{1}{729^k} \left( \frac{243}{(12k+1)^2} - \frac{405}{(12k+2)^2} - \frac{81}{(12k+4)^2} \right)
\]
\[
\log \left( \frac{9}{10} \right) = -\frac{1}{10} \sum_{k=0}^{\infty} \frac{1}{10^k}
\]
\[
\log \left( \frac{1111111111}{387420489} \right) = \frac{1}{10^8} \sum_{k=0}^{\infty} \frac{1}{1010^k} \left( \frac{10^8}{10k+1} + \frac{10^7}{10k+2} + \frac{10^6}{10k+3} \right)
\]
\[
\log \left( \frac{781}{256} \right) \left( \frac{57 - 5\sqrt{5}}{57 + 5\sqrt{5}} \right)^{\frac{5}{2}} = \sum_{k=0}^{\infty} \frac{1}{5^k} \left( \frac{5}{5k+2} + \frac{1}{5k+3} \right)
\]

Table 3.7. Nonbinary BBP-type formulas.

Gaussian primes dividing \( p \), and where we require \( 0 < \Im(p) < R(p) \) to make the definition of \( \theta_p \) unambiguous. Note that

\[
\theta_p(wz) = \theta_p(w) + \theta_p(z). \tag{3.51}
\]

Given \( \kappa \in R \), with \( 2 \leq b \in Z \) and \( b \) not a proper power, we say that \( \kappa \) has a \( Z \)-linear or \( Q \)-linear \textit{Machin-type BBP arctangent formula} to the
3.7. Does Pi Have a Nonbinary BBP Formula?

base \( b \) if and only if \( \kappa \) can be written as a \( \mathbb{Z} \)-linear or \( \mathbb{Q} \)-linear combination (respectively) of generators of the form

\[
\arctan \left( \frac{1}{b^m} \right) = 3 \log \left( 1 + \frac{i}{b^m} \right) = b^m \sum_{k=0}^{\infty} \frac{(-1)^k}{b^{2mk}(2k+1)}.
\]

(3.52)

We will also use the following theorem, first proved by Bang in 1886:

**Theorem 3.6.** The only cases where \( b^m - 1 \) has no primitive prime factor(s) are when \( b = 2, m = 6, b^m - 1 = 3^2 \cdot 7 \); and when \( b = 2^N - 1, N \in \mathbb{Z}, m = 2, b^m - 1 = 2^{N+1}(2^{N-1} - 1) \).

We can now state the main result of this section:

**Theorem 3.7.** Given \( b > 2 \) and not a proper power, then there is no \( \mathbb{Q} \)-linear Machin-type BBP arctangent formula for \( \pi \).

**Proof.** It follows immediately from the definition of a \( \mathbb{Q} \)-linear Machin-type BBP arctangent formula that any such formula has the form

\[
\pi = \frac{1}{n} \sum_{m=1}^{M} n_m 3 \log(b^m - i)
\]

(3.53)

where \( n > 0 \in \mathbb{Z}, n_m \in \mathbb{Z}, \text{ and } M \geq 1, n_M \neq 0 \). This implies that

\[
\prod_{m=1}^{M} (b^m - i)^{n_m} \in e^{n \pi} \mathbb{Q}^x = \mathbb{Q}^x
\]

(3.54)

For any \( b > 2 \) and not a proper power it follows from Bang’s Theorem that \( b^{4M} - 1 \) has a primitive prime factor, say \( p \). Furthermore, \( p \) must be odd, since \( p = 2 \) can only be a primitive prime factor of \( b^m - 1 \) when \( b \) is odd and \( m = 1 \). Since \( p \) is a primitive prime factor, it does not divide \( b^{2M} - 1 \), and so \( p \) must divide \( b^{2M} + 1 = (b^M + i)(b^M - i) \). We cannot have both \( p | b^M + i \) and \( p | b^M - i \), since this would give the contradiction that \( p | (b^M + i) - (b^M - i) = 2i \). It follows that \( p \equiv 1 \pmod{4} \), and that \( p \) factors as \( p = \overline{p} \) over \( \mathbb{Z}[i] \), with exactly one of \( p, \overline{p} \) dividing \( b^M - i \). Referring to the definition of \( \theta \), we see that we must have \( \theta(p)(b^M - i) \neq 0 \). Furthermore, for any \( m < M \), neither \( p \) nor \( \overline{p} \) can divide \( b^m - i \) since this would imply \( p | b^{4m} - 1, 4m < 4M \), contradicting the fact that \( p \) is a primitive prime factor of \( b^{4M} - 1 \). So for \( m < M \), we have \( \theta(p)(b^m - i) = 0 \). Referring to equation (3.53), using Equation (3.51) and the fact that \( n_M \neq 0 \), we get...
Thus our assumption that there was a $b$-ary Machin-type BBP arctangent formula for $\pi$ must be false.

3.8 Commentary and Additional Examples

1. The ENIAC Integrator and Calculator. ENIAC, built in 1946 at the University of Pennsylvania, had 18,000 vacuum tubes, 6,000 switches, 10,000 capacitors, 70,000 resistors, 1,500 relays, was 10 feet tall, occupied 1,800 square feet, and weighed 30 tons. ENIAC could perform 5,000 arithmetic operations per second—1,000 times faster than any earlier machine, but a far cry from today’s leading-edge microprocessors, which can perform more than four billion operations per second. The first stored-memory computer, ENIAC could store 200 digits, which again is a far cry from the hundreds of megabytes in a modern personal computer system. Data flowed from one accumulator to the next, and after each accumulator finished a calculation, it communicated its results to the next in line. The accumulators were connected to each other manually. A photo is shown in Figure 3.3.

2. Four approximations to pi. Here are two well known, but fascinating, approximations to $\pi$:

$$\pi \approx \frac{3}{\sqrt{163}} \log (640320),$$
correct to 15 decimal places, and

$$\pi \approx \frac{3}{\sqrt{64}}, \log (5280),$$
correct to 9 decimal places. Both rely on somewhat deeper number theory (see Section 1.4 in the second volume). Here are two nice algebraic $\pi$ approximations:

$$\pi \approx 66 \frac{\sqrt{2}}{33 \sqrt{29} - 148}$$
3.8. Commentary and Additional Examples

and

\[ \pi \approx \frac{63}{25} \frac{17 + 15 \sqrt{5}}{7 + 15 \sqrt{5}}. \]

3. **An arctan series for pi.** Find rational coefficients \( a_i \) such that the identity

\[
\pi = a_1 \arctan \frac{1}{390112} + a_2 \arctan \frac{1}{485298} + a_3 \arctan \frac{1}{683982} + a_4 \arctan \frac{1}{1984933} + a_5 \arctan \frac{1}{2478328} + a_6 \arctan \frac{1}{3449051} + a_7 \arctan \frac{1}{18975991} + a_8 \arctan \frac{1}{22709274} + a_9 \arctan \frac{1}{24208144} + a_{10} \arctan \frac{1}{201229582} + a_{11} \arctan \frac{1}{2189376182}
\]
holds [7 pg. 75]. Also show that an identity with even simpler coefficients exists if \( \arctan 1/239 \) is included as one of the terms on the RHS. *Hint:* Use an integer relation program (see Section 6.3), or try the tools at one of these sites: http://www.cecm.sfu.ca/projects/IntegerRelations or http://www.experimentalmath.info.

4. **Ballantine’s series for \( \pi \).** A formula of Euler for \( \text{arccot} \) is

\[
x \sum_{n=0}^{\infty} \frac{(n!)^2 4^n}{(2n+1)! (x^2 + 1)^{n+1}} = \arctan \left( \frac{1}{x} \right). \tag{3.56}
\]

As observed by Ballantine in 1939, (34) this allows one to rewrite the variant of Machin’s formula, used by Guilloud and Bouyer in 1973 to compute a million digits of \( \pi \),

\[
\frac{\pi}{4} = 12 \arctan \left( \frac{1}{18} \right) + 8 \arctan \left( \frac{1}{57} \right) - 5 \arctan \left( \frac{1}{239} \right) \tag{3.57}
\]

in the neat form

\[
\pi = 864 \sum_{n=0}^{\infty} \frac{(n!)^2 4^n}{(2n+1)! 325^{n+1}} + 1824 \sum_{n=0}^{\infty} \frac{(n!)^2 4^n}{(2n+1)! 3250^{n+1}}
- 20 \arctan \left( \frac{1}{239} \right), \tag{3.58}
\]

where the terms of the second series are just decimal shifts of the terms of the first.

5. **Convergence rates for \( \pi \) formulas.** Analyze the rates of convergence of Archimedes iteration (3.1), the Salamin-Brent iteration (3.16), the Borwein cubic iteration (3.17) and the Borwein quartic iteration (3.18), by means of explicit computations. Use the high-precision arithmetic facility built into *Maple* or *Mathematica*, or write your own C++ or Fortran-90 code using the ARPREC arbitrary precision software available at http://www.experimentalmath.info, or the GNU multiprecision software available at http://www.gnu.org/software/gmp/gmp.html. Such iterations are discussed more in Sections 5.6.2 and 5.6.3.

6. **Biblical \( \pi \).** As noted in Section 3.1, the Biblical passages 1 Kings 7:23 and 2 Chronicles 4:2 indicate that \( \pi = 3 \). In spite of the fact the context of these verses clearly suggests an informal approximation, not a precise statement of mathematical fact, this discrepancy has
been a source of consternation among Biblical literalists for centuries. For example, an 18th-century German Bible commentary attempted to explain away this discrepancy using the imaginative (if pathetic) suggestion that the circular pool in Solomon’s temple (clearly described in 2 Chron. 4:2 as “round in compass”) was instead hexagonal in shape [33 pg. 75–76]. Even today, some are still unwilling to accept that the Bible could simply be mistaken here. One evangelical scholar, for example, writes:

However, the recorded dimensions are still no problem if we consider the shape of the vessel. In 1 Kings 7:26, we read that its “brim was made like the brim of a cup, as a lily blossom.” Hence, the sea was not a regular cylinder, but had an outward curving rim. Although we do not know the exact points on the vessel where the measurements were taken, the main part of the sea always will be somewhat smaller than the 10 cubits measured “from brim to brim.” [150]

Another geometric difficulty in these Biblical passages is that 1 Kings 7:26 (three verses after it gives its dimensions) gives a volume of 2,000 “baths” for the basin, while 2 Chron. 4:5 gives the figure 3,000 baths. 2 Chron. 4:2 gives the height of the basin as five cubits. Using the accepted conversions that one “cubit” is roughly 46 cm, and that one “bath” is roughly 23 liters, then assuming Solomon’s pool was cylindrical in shape, we obtain an actual volume of roughly 1660 baths. If the basin was rounded on the bottom, then its volume was even lower than this.

7. **Exponentiation of pi.** Arguably the most accessible transcendental number to compute is \( e^\pi \). The following iteration computes \( D \) digits in \( \log(D) \) steps.

**Algorithm 3.8.** *Computation of \( \exp(\pi) \).*

Set \( k_0 = 1/\sqrt{2} \) and for \( n < N \) iterate

\[
k'_n = \sqrt{1 - k_n^2}, \quad k_{n+1} = \frac{1 - k'_n}{1 + k'_n}.
\]

Then return

\[
\left( \frac{k_N}{4} \right)^{-1/2^N}.
\]

Some care needs to be taken with guard digits. □
8. **Algorithms for Gamma values.** An algorithm for π may be viewed as an algorithm for \( \Gamma \left( \frac{1}{2} \right) \), and there is a quite analogous iteration for \( \Gamma \) at the values 1/3, 2/3, 1/4, 3/4, 1/6, and 5/6. This, in turn, allows rapid computation of \( \Gamma \left( \frac{k}{24} \right) \), for all integer \( k \). We illustrate with:

**Algorithm 3.9. Computation of \( \Gamma \left( \frac{1}{4} \right) \).**

Let \( x_0 = 2^{1/2}, y_1 = 2^{1/4} \). Let

\[
\begin{align*}
x_{n+1} &= \frac{\sqrt{x_n} + 1/\sqrt{x_n}}{2} \quad (3.59) \\
y_{n+1} &= \frac{y_n \sqrt{x_n} + 1/\sqrt{x_n}}{y_n + 1}. \quad (3.60)
\end{align*}
\]

Then

\[
\Gamma^4 \left( \frac{1}{4} \right) = 16 \left( 1 + \sqrt{2} \right)^3 \prod_{n=1}^{\infty} x_n^{-1} \left( \frac{1 + x_n}{1 + y_n} \right)^3.
\]

This yields a quadratically convergent iteration for \( \Gamma \left( \frac{1}{4} \right) \). \( \square \)

No such iteration is known for \( \Gamma \left( \frac{1}{5} \right) \); see [49, 45].

9. **An integral representation of Euler’s constant.** While it is known that \( \Gamma \left( \frac{1}{3} \right) \) and \( \Gamma \left( \frac{1}{4} \right) \) are transcendental, the status of Euler’s constant

\[
\gamma = \lim_{n \to \infty} \sum_{k=1}^{n} \frac{1}{k} - \log(n) \quad (3.61)
\]

is unsettled.

**Problem:** Show that

\[
\gamma = \int_{0}^{\infty} \left( \frac{1}{e^t - 1} - \frac{1}{t e^t} \right) dt.
\]

10. **Computation of Euler’s constant.** Perhaps the most efficient method of computation, due to Brent and MacMillan ([49 pg. 336]), is based on Bessel function identities. It allows one to show that if \( \gamma \) is rational it must have a denominator with millions of digits. The underlying identity, known to Euler, is

\[
\gamma + \log(z/2) = \frac{S_0(z) - K_0(z)}{I_0(z)} \quad (3.62)
\]
where $I_\nu(z) = \sum_{k=0}^{\infty} (z/2)^{2k+\nu}/(k! \Gamma(k+\nu+1))$, while $K_\nu(z) = \partial I_\nu(0)/\partial \nu$ and $S_\nu(z) = \sum_{k=0}^{\infty} (\sum_{j=1}^{k} 1/j) (z/2)^{2k}/(k!)^2$.

An algorithm follows from knowing the first terms of the asymptotic expansion for $K_\nu$ and $I_\nu$. It is

**Algorithm 3.10. Computation of $K_\nu$ and $I_\nu$:**

\begin{align*}
A_0 &= -\log(n), B_0 = 1, U_0 = A_0, V_0 = 1, \text{ and for } k = 1, 2, \ldots , \\
B_k &= B_{k-1}n^2/k^2, \quad A_k = (A_{k-1}n^2/k + B_k)/k, \\
U_k &= U_{k-1} + A_k, \quad V_k = V_{k-1} + B_k.
\end{align*}

Terminate when $U_k$ and $V_k$ no longer change, and return $\gamma \approx U_k/V_k$.

With $\log(n)$ computed efficiently, this scheme takes $O(D)$ storage and approximately $2.07 D$ steps to compute $\gamma$ to $D$ decimal places.

11. **Buffon’s needle.** Suppose we have a lined sheet of paper, and a needle that is precisely as long as the distance between the lines. Compute the probability that the needle “thrown at random” on the sheet of paper will lie on a line. Answer: $2/\pi$. Although this is certainly not a good way to calculate $\pi$ (millions of trials would be required to obtain just a few digits), it is an instructive example of how $\pi$ arises in unlikely settings (see also the next two exercises). Some additional discussion of this problem, plus a computer-based tool that allows one to perform these trials, is available at the URL [http://www.mste.uiuc.edu/reese/buffon/buffon.html](http://www.mste.uiuc.edu/reese/buffon/buffon.html).

12. **Putnam problem 1993-B3.** If two real numbers $x$ and $y$ are generated uniformly at random in $(0,1)$, what is the probability that the nearest integer to $x/y$ is even? **Hint:** Ignoring negligible events, for this to occur either $0 < x/y < 1/2$ or $(4n-1)/2 < x/y < (4n+1)/2$. The first occurs in a triangle of area $1/4$ and the subsequent in triangles of area $1/(4n-1) - 1/(4n+1)$. Now apply the Gregory-Leibniz formula. Answer: The probability is $(5 - \pi)/4 \approx 0.4646018$.

13. **Number-theory probabilities.** Prove (a) The probability that an integer is square-free is $6/\pi^2$. (b) The probability that two integers are relatively prime is also $6/\pi^2$. This is a good example of $\pi$ appearing in a number-theory setting. See [109].

14. **The irrationality of $\pi$.** We reproduce in extenso Ivan Niven’s 1947 very concise proof that $\pi$ is irrational [158].
Let \( \pi = a/b \), the quotient of positive integers. We define the polynomials
\[
f(x) = \frac{x^n(a - bx)^n}{n!}
\]
\[
F(x) = f(x) - f^{(2)}(x) + f^{(4)}(x) - \cdots + (-1)^n f^{(2n)}(x),
\]
the positive integer \( n \) being specified later. Since \( n!f(x) \) has integral coefficients and terms in \( x \) of degree not less than \( n \), \( f(x) \) and its derivatives \( f^{(j)}(x) \) have integral values for \( x = 0 \); also for \( x = \pi = a/b \), since \( f(x) = f(a/b - x) \). By elementary calculus we have
\[
\frac{d}{dx}\{F'(x) \sin x - F(x) \cos x\} = F''(x) \sin x + F(x) \sin x = f'(x) \sin x
\]
and
\[
\int_0^\pi f(x) \sin x dx = [F'(x) \sin x - F(x) \cos x]|_0^\pi = F(\pi) + F(0). (3.64)
\]
Now \( F(\pi) + F(0) \) is an integer, since \( f^{(j)}(0) \) and \( f^{(j)}(\pi) \) are integers. But for \( 0 < x < \pi \),
\[
0 < f(x) \sin x < \frac{\pi^n a^n}{n!},
\]
so that the integral in (3.64) is positive but arbitrarily small for \( n \) sufficiently large. Thus (3.64) is false, and so is our assumption that \( \pi \) is rational. \( \square \)

This proof gives a good taste of the ingredients of more subtle irrationality and transcendence proofs.

15. **A spigot algorithm for e and \( \pi \).** A spigot method for a numerical constant is one that can produce digits one by one (“drop by drop”) \[ ^{[169]} \]. This is especially easy for \( e \) as carries are not a big issue.

(a) The following algorithm, due to Rabinowitz and Wagon, generates successive digits of \( e \). Initialize an array \( A \) of length \( n + 1 \) to 1. Then repeat the following \( n - 1 \) times: (a) multiply each entry in \( A \) by ten; (b) Starting from the right, reduce the \( i \)-th entry of \( A \) modulo \( i + 1 \), carrying the quotient of the division one place left. The final quotient produced is the next digit of \( e \). This algorithm is based on the following formula, which is simply a restatement of \( e = \sum 1/i! \).

\[
e = 1 + \frac{1}{1} \left( 1 + \frac{1}{2} \left( 1 + \frac{1}{3} \left( 1 + \frac{1}{4} \left( 1 + \frac{1}{5} (1 + \cdots) \right) \right) \right) \right).
\]
3.8. Commentary and Additional Examples

(b) Implement a parallel spigot algorithm for \( \pi \), based on showing that:

\[
\pi = 2 + \frac{1}{3} \left( 2 + \frac{2}{5} \left( 2 + \frac{3}{7} \left( 2 + \cdots \left( 2 + \frac{k}{2k+1} + \cdots \right) \right) \right) \right).
\]

The last term can be approximated by \( 2 + 4k/(2k+1) \) where \( k = \log_2(10) n \) to produce \( n \) digits of \( \pi \) “drop by drop.” If one wishes to run the algorithm without a specified end, one must take more care.

One may view the iteration (4.7), which we will study in Chapter 4, as a spectacular (albeit unproven) spigot algorithm for \( \pi \) base 16.

16. Wagon’s BBP identity. Determine the range of validity of the following identity, which is due to Stan Wagon:

\[
\pi + 4 \arctan z + 2 \log \left( \frac{1 - 2z - z^2}{z^2 + 1} \right) = \sum_{k=0}^{\infty} \frac{1}{16^k} \left( \frac{4(z + 1)^{1+8k}}{1 + 8k} - \frac{2(z + 1)^{4+8k}}{4 + 8k} - \frac{(z + 1)^{5+8k}}{5 + 8k} - \frac{(z + 1)^{6+8k}}{6 + 8k} \right).
\]

17. Monte Carlo calculation of \( \pi \). Monte Carlo simulation was pioneered during the Manhattan project by Stanislaw Ulam and others, who recognized that this scheme permitted simulations beyond the reach of conventional methods on the systems then available. We illustrate here a Monte Carlo calculation of \( \pi \), which is a poor method to compute \( \pi \), but illustrative of this general class of computation. Nowadays, Monte Carlo methods are quite popular because they are well suited to parallel computation on systems such as “Beowulf” clusters.

(a) Design and implement a Monte Carlo simulation for \( \pi \), based on generating pairs of uniformly distributed numbers in the unit square and testing whether they lie inside the unit circle. Use the pseudorandom number generator \( x_0 = 314159 \) and \( x_n = cx_{n-1} \mod 2^{32} \), where \( c = 5^{5} = 1953125 \). This generator is of the well known class of linear congruential generators and has period \( 2^{30} \) [130, pg. 21]. It can be easily implemented on a computer using IEEE 64-bit “double” datatype, since the largest integer that can arise here is less than \( 2^{33} \). Variations with longer periods can easily be designed, although the implementation is not as convenient. The results of this generator are normalized, by \( 2^{32} \) in this case, to produce results in the unit interval.
(b) Extend your program to run on a parallel computer system, with the property that your parallel program generates the same overall scheme of pseudorandom numbers, and thus gets the same result for \( \pi \), as a serial implementation (you may for convenience assume that \( n \), the total number of pseudorandom numbers generated, is evenly divisible by \( p \), the number of processors). This is a very desirable feature of a parallel program, because it allows you to certify your parallel results by comparing them with a conventional single-processor run, and it permits you to take advantage of a range of system sizes. \textit{Hint}: Design the program so that processor \( k \) (where processors are numbered from 0 to \( p - 1 \)) generates the \( m = n/p \) members of the sequence \((x_{km}, x_{km+1}, x_{km+2}, \ldots, x_{km+m-1})\). Note that the starting value \( x_{km} \) for processor \( k \) can be directly computed as \( x_{km} = 5^{\text{km}} x_0 \mod 2^{32} \). This exponentiation modulo \( 2^{32} \) may be performed by using Algorithm 3.0 implemented with 128-bit floating-point or “double-double” arithmetic (see Section 6.2.1).

(c) Generate the following sequence of pseudorandom numbers and experimentally determine what distribution they satisfy (i.e., by computing means, standard deviations, graphs, etc.): Let \( x_1 \) and \( x_2 \) be a pair of uniform \((0, 1)\) pseudorandom numbers generated as described above. Set \( v = \sqrt{x_1^2 + x_2^2} \) and \( w = \sqrt{-2 \log v/v} \). Then produce the results \( y_1 = wx_1 \) and \( y_2 = wx_2 \).

18. \textbf{Life of Pi}. At the end of his story, Piscine (Pi) Molitor \[152\] pp.316–7 writes

I am a person who believes in form, in harmony of order. Where we can, we must give things a meaningful shape. For example—I wonder—could you tell my jumbled story in exactly one hundred chapters, not one more, not one less? I’ll tell you, that’s one thing I hate about my nickname, the way that number runs on forever. It’s important in life to conclude things properly. Only then can you let go.

We may not share the sentiment, but we should celebrate that Pi knows \( \pi \) to be irrational.
4

Normality of Numbers

Anyone who wants to make a name for himself can examine the major issue of whether \( \pi \) is *normal*, or perhaps more accurately, whether \( \pi \) is *not normal*.

– Jörg Arndt and Christoph Haenel, *Pi Unleashed*, 2001

In this chapter, we address a fundamental problem of mathematics, a paradox of sorts: Whereas on one hand it can be proven that “almost all” real numbers are normal, and whereas it appears from experimental analysis that many of the fundamental constants of mathematics are normal to commonly used number bases, as yet there are no proofs, nor even any solid reason why we should observe this behavior. What we shall show here is that the theory of BBP constants, which as we have seen is a classic case study of experimental mathematics in action, opens a pathway into the investigation of normality, and in fact has already yielded some intriguing results.

4.1 Normality: A Stubborn Question

Given a real number \( \alpha \) and an integer \( b > 2 \), we say that \( \alpha \) is \( b \)-normal or *normal base \( b \)* if every sequence of \( k \) consecutive digits in the base-\( b \) expansion of \( \alpha \) appears with limiting frequency \( b^{-k} \). In other words, if a constant is 10-normal, then the limiting frequency of “3” (or any other single digit) in its decimal expansion is 1/10, the limiting frequency of “58” (or any other two-digit pair) is 1/100, and so forth. We say that a real number \( \alpha \) is *absolutely normal* if it is \( b \)-normal for all integers \( b > 1 \) simultaneously.

In spite of these strong conditions, it is well known from measure theory that the set of absolutely normal real numbers in the unit interval has measure one, or in other words, that almost all real numbers are absolutely normal (see Exercise 1 at the end of this chapter). Further, from
numerous analyses of computed digits, it appears that many of the fundamental constants of mathematics are normal to commonly used number bases. By “fundamental constants,” we include \( \pi, e, \sqrt{2}, \) the golden mean \( \tau = (1 + \sqrt{5})/2, \) as well as \( \log n \) and the Riemann zeta function \( \zeta(n) \) for positive integers \( n > 1, \) and many others. For example, it is a reasonable conjecture that every irrational algebraic number is absolutely normal, since there is no known example of an irrational algebraic number whose decimal expansion (or expansion in any other base) appears to have skewed digit-string frequencies.

Decimal values are given for a variety of well known mathematical constants in Table 4.1 [65, 94]. In addition to the widely recognized constants such as \( \pi \) and \( e, \) we have listed Catalan’s constant \( G, \) Euler’s constant \( \gamma, \) an evaluation of the elliptic integral of the first kind \( K(1/\sqrt{2}), \) an evaluation of an elliptic integral of the second kind \( E(1/\sqrt{2}), \) Feigenbaum’s \( \alpha \) and \( \delta \) constants, Khintchine’s constant \( K, \) and Madelung’s constant \( M. \) Binary values for some of these constants, as well as Chaitin’s \( \Omega \) constant (from the field of computational complexity) [65], are given in Table 4.2. As you can see, none of the expansions in either table exhibits any evident “pattern.”

The digits of \( \pi \) have been studied more than any other single constant, in part because of the widespread fascination with \( \pi. \) Along this line, Yasumasa Kanada of the University of Tokyo has tabulated the number of occurrences of the ten decimal digits “0” through “9” in the first one trillion decimal digits of \( \pi. \) These counts are shown in Table 4.3. For reasons given in Section 3.4, binary (or hexadecimal) digits of \( \pi \) are also of considerable interest. To that end, Kanada has also tabulated the number of occurrences of the 16 hexadecimal digits “0” through “F,” as they appear in the first one trillion hexadecimal digits. These counts are shown in Table 4.4. As you can see, both the decimal and hexadecimal single-digit counts are entirely reasonable.

Some readers may be amused by the LBNL PiSearch utility, which is available at [http://pisearch.lbl.gov](http://pisearch.lbl.gov). This online tool permits one to enter one’s name (or any other modest-length alphabetic string, or any modest-length hexadecimal string) and see if it appears encoded in the first several billion binary digits of \( \pi. \) Along this line, a graphic based on a random walk of the first million decimal digits of \( \pi, \) courtesy of David and Gregory Chudnovsky, is shown in Figure 4.1 (see Color Plate VIII). It maps the digit stream to a surface in ways similar to those used by Mandelbrot and others.

As we mentioned in Section 3.2, the question of whether \( \pi, \) in particular, or, say, \( \sqrt{2}, \) is normal or not has intrigued mathematicians for centuries. But in spite of centuries of effort, not a single one of the fundamental
4.1. Normality: A Stubborn Question

Table 4.1. Decimal values of various mathematical constants.

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sqrt{2}$</td>
<td>1.4142135623730950488...</td>
</tr>
<tr>
<td>$\sqrt{3}$</td>
<td>1.7320508075688772935...</td>
</tr>
<tr>
<td>$\sqrt{5}$</td>
<td>2.2360677774999999999964...</td>
</tr>
<tr>
<td>$\phi = \sqrt{5} + 1 \over 2$</td>
<td>0.6180339887498948482...</td>
</tr>
<tr>
<td>$1/\pi$</td>
<td>0.31830988618379067153...</td>
</tr>
<tr>
<td>$e$</td>
<td>2.7182818284590452354...</td>
</tr>
<tr>
<td>$1/e$</td>
<td>0.36787944117144232160...</td>
</tr>
<tr>
<td>$e^\pi$</td>
<td>23.140692632779269007...</td>
</tr>
<tr>
<td>$\log 2$</td>
<td>0.69314718055994530942...</td>
</tr>
<tr>
<td>$\log 10$</td>
<td>2.3025850929940456840...</td>
</tr>
<tr>
<td>$\log_{10} 2$</td>
<td>0.30102999566398119522...</td>
</tr>
<tr>
<td>$\log_{10} 3$</td>
<td>0.584962500721156815...</td>
</tr>
<tr>
<td>$\zeta(2)$</td>
<td>0.6449340668482264365...</td>
</tr>
<tr>
<td>$\zeta(3)$</td>
<td>0.2020569031595942854...</td>
</tr>
<tr>
<td>$\zeta(5)$</td>
<td>0.103692775143369263...</td>
</tr>
<tr>
<td>$G$</td>
<td>0.91596559417721901505...</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>0.57721566490153286061...</td>
</tr>
<tr>
<td>$\Gamma(1/2)$</td>
<td>1.7724538509055160273...</td>
</tr>
<tr>
<td>$\Gamma(1/3)$</td>
<td>2.667783534707746337...</td>
</tr>
<tr>
<td>$\Gamma(1/4)$</td>
<td>3.6569909221083121...</td>
</tr>
<tr>
<td>$K(1/\sqrt{2})$</td>
<td>1.854074573013719184...</td>
</tr>
<tr>
<td>$E(1/\sqrt{2})$</td>
<td>1.35604388104767550525...</td>
</tr>
<tr>
<td>$\omega_f$</td>
<td>4.669201609102990...</td>
</tr>
<tr>
<td>$\delta_f$</td>
<td>2.502997875595892...</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>2.6854520910653064453...</td>
</tr>
<tr>
<td>$\log_{10} \gamma$</td>
<td>1.4720645694691821903...</td>
</tr>
</tbody>
</table>

Table 4.2. Binary values of various mathematical constants.
### 4. Normality of Numbers

<table>
<thead>
<tr>
<th>Digit</th>
<th>Occurrences</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>99999485134</td>
</tr>
<tr>
<td>1</td>
<td>9999945664</td>
</tr>
<tr>
<td>2</td>
<td>10000048057</td>
</tr>
<tr>
<td>3</td>
<td>99999787805</td>
</tr>
<tr>
<td>4</td>
<td>100000357857</td>
</tr>
<tr>
<td>5</td>
<td>99999671008</td>
</tr>
<tr>
<td>6</td>
<td>99999807503</td>
</tr>
<tr>
<td>7</td>
<td>99999818723</td>
</tr>
<tr>
<td>8</td>
<td>100000791469</td>
</tr>
<tr>
<td>9</td>
<td>99999854780</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>1000000000000</strong></td>
</tr>
</tbody>
</table>

**Table 4.3.** Statistics for the first trillion decimal digits of \( \pi \).

<table>
<thead>
<tr>
<th>Digit</th>
<th>Occurrences</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>62499881108</td>
</tr>
<tr>
<td>1</td>
<td>62500212206</td>
</tr>
<tr>
<td>2</td>
<td>62499924780</td>
</tr>
<tr>
<td>3</td>
<td>62500188844</td>
</tr>
<tr>
<td>4</td>
<td>62499807368</td>
</tr>
<tr>
<td>5</td>
<td>62500007205</td>
</tr>
<tr>
<td>6</td>
<td>62499925426</td>
</tr>
<tr>
<td>7</td>
<td>62499878794</td>
</tr>
<tr>
<td>8</td>
<td>62500216752</td>
</tr>
<tr>
<td>9</td>
<td>62500120671</td>
</tr>
<tr>
<td>A</td>
<td>62500266095</td>
</tr>
<tr>
<td>B</td>
<td>62499955595</td>
</tr>
<tr>
<td>C</td>
<td>62500188610</td>
</tr>
<tr>
<td>D</td>
<td>62499613666</td>
</tr>
<tr>
<td>E</td>
<td>62499875079</td>
</tr>
<tr>
<td>F</td>
<td>62499937801</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>1000000000000</strong></td>
</tr>
</tbody>
</table>

**Table 4.4.** Statistics for the first trillion hexadecimal digits of \( \pi \).
constants of mathematics has ever been proven to be $b$-normal for any integer $b$, much less for all integer bases simultaneously. And this is not for lack of trying—some very good mathematicians have seriously investigated this problem, but to no avail. Even much weaker results, such as the digit “1” appears with nonzero limiting frequency in the binary expansion of $\pi$, and the digit “5” appears infinitely often in the decimal expansion of $\sqrt{2}$, have heretofore remained beyond the reach of modern mathematics.

One result in this area is the following. Let $f(n) = \sum_{1 \leq j \leq n} \lfloor \log_{10} j \rfloor$. Then the Champernowne number,

$$\sum_{n=1}^{\infty} \frac{n}{10^{n+f(n)}} = 0.12345678910111213141516171819202122232425\ldots,$$

where the positive integers are concatenated in a decimal value, is known to be 10-normal (See Exercise 5). There are similar constants and normality results for other number bases. However, no one, to the authors’ knowledge, has ever argued that this constant and its relatives are “natural” or “fundamental” constants.

Consequences of a proof in this area would definitely be interesting. For starters, such a proof would immediately provide an inexhaustible source of provably reliable pseudorandom numbers for numerical or scientific experimentation. We also would obtain the mind-boggling but uncontestable
consequence that if $\pi$, for example, is shown to be 2-normal, then the entire text of the Bible, the Koran and the works of William Shakespeare, as well as the full \LaTeX\ source text for this book, must all be contained somewhere in the binary expansion of $\pi$, where consecutive blocks of eight bits (two hexadecimal digits) each represent one ASCII character. Unfortunately, this would not be much help to librarians or archivists, since every conceivable misprint of each of these books would also be contained in the binary digits of $\pi$.

Before continuing, we should mention the “first digit” principle, also known as Benford’s principle. In the 1880s, Simon Newcomb observed a pattern in the first digits of logarithm tables: A “1” is significantly more likely to occur than “2,” a “2” more than a “3,” and so on. In other words, the collection of first digits of data in logarithm tables certainly does not reflect the statistics expected of 10-normal numbers. In the 20th century, Frank Benford rediscovered this phenomenon, noting that it applies to many types of numerical data, ranging from values of physical constants to census data to the stock market. One can deduce this principle by observing that natural laws surely cannot be dependent on our choice of units, and thus must be scale-independent. This suggests that we view numerical data on a logarithmic scale. In the logarithmic sense, a leading “1” appears roughly 30% of the time (since $\log_{10} 2 - \log_{10} 1 = 0.30102999\ldots$), a “2” appears roughly 17.6% of the time (since $\log_{10} 3 - \log_{10} 2 = 0.1760912\ldots$), and so on. More recently scientists have applied Benford’s principle in diverse ways, including fraud detection in business accounting [117].

4.2 BBP Constants and Normality

Until recently, the BBP formulas mentioned in Sections 3.4 and 3.6 were assigned by some to the realm of “recreational” mathematics—interesting but of no serious consequence. But the history of mathematics has seen many instances where results once thought to be idle curiosities were later found to have significant consequences. This now appears to be the case with the theory of BBP-type constants.

What we shall establish below, in a nutshell, is that the 16-normality of $\pi$ (which, of course, is equivalent to the 2-normality of $\pi$), as well as the normality of numerous other irrational constants that possess BBP-type formulas, can be reduced to a certain plausible conjecture in the theory of chaotic sequences. At this time we do not know the full implications of this result. It may be the first salvo in the resolution of this age-old mathematical question, or it may be merely a case of reducing one very difficult mathematical problem to another. But at the least, this result
appears to lay out a structure—a “roadmap” of sorts—for the analysis of this question. Thus it seems worthy of investigation.

We shall also establish that a certain well-defined class of real numbers, uncountably infinite in number, is indeed $b$-normal for certain bases $b$. This result is not dependent on any unproven conjecture. We will also present some results on the digit densities of algebraic irrationals. All of these recent results are direct descendants of the theory of BBP-type constants that we have presented in Sections 3.4 and 3.6.

The results for BBP-type constants derive from the following observation, which was given in a recent paper by one of the present authors and Richard Crandall [24]. Here we define the norm $||\alpha||$ for $\alpha \in [0, 1)$ as $||\alpha|| = \min(\alpha, 1 - \alpha)$. With this definition, $||\alpha - \beta||$ measures the shortest distance between $\alpha$ and $\beta$ on the unit circumference circle in the natural way. Suppose $\alpha$ is given by a BBP-type formula, namely

$$\alpha = \sum_{k=0}^{\infty} \frac{p(k)}{b^k q(k)},$$

where $p$ and $q$ are polynomials with integer coefficients, with $0 \leq \deg p < \deg q$, and with $q$ having no zeroes at nonnegative integer arguments. Now define the recursive sequence $(x_n)$ as $x_0 = 0$, and

$$x_n = \left\{ bx_{n-1} + \frac{p(n)}{q(n)} \right\},$$

where the notation $\{ \cdot \}$ denotes the fractional part as before. Recall from Section 3.4 that we can write the base-$b$ expansion of $\alpha$ beginning at position $n+1$, which we denote $\alpha_n$, as

$$\alpha_n = \{ b^n \alpha \} = \left\{ \sum_{k=0}^{\infty} \frac{b^{n-k} p(k)}{q(k)} \right\}$$

$$= \left\{ \left\{ \sum_{k=0}^{n} \frac{b^{n-k} p(k)}{q(k)} \right\} + \sum_{k=n+1}^{\infty} \frac{b^{n-k} p(k)}{q(k)} \right\}.$$  

(4.3)

Now observe that the sequence $(x_n)$ generates the first part of this expression. In particular, given $\epsilon > 0$, assume that $n$ is sufficiently large such that $p(k)/q(k) < \epsilon$ for all $k \geq n$. Then we can write, for all sufficiently large $n$,

$$||x_n - \alpha_n|| \leq \left| \sum_{k=n+1}^{\infty} \frac{b^{n-k} p(k)}{q(k)} \right|$$

$$\leq \epsilon \sum_{k=n+1}^{\infty} b^{n-k} = \frac{\epsilon}{b-1} \leq \epsilon.$$  

(4.4)
With this argument, we have established the following, which we observe is also true if the expression \( p(k)/q(k) \) is replaced by any more general sequence \( r(k) \) that tends to zero for large \( k \):

**Theorem 4.11.** Let \( \alpha \) be a BBP-type constant as defined above, with \( \alpha_n \) the base-\( b \) expansion of \( \alpha \) beginning at position \( n + 1 \), and \( (x_n) \) the BBP sequence associated with \( \alpha \), as given in (4.2) above. Then \( |x_n - \alpha_n| \to 0 \) as \( n \to \infty \).

In other words, the BBP sequence associated with \( \alpha \), as given in Formula (4.2), is a close approximation to the sequence \( (\alpha_n) \) of shifted digit expansions, so much so that if one has a property such as equidistribution in the unit interval, then the other does also (this will be made precise in Section 4.5). We now state a hypothesis, which is believed to be true, based on experimental evidence, but which is not yet proven:

**Hypothesis 4.12.** (Bailey-Crandall). Let \( p(x) \) and \( q(x) \) be polynomials with integer coefficients, with \( 0 \leq \deg p < \deg q \), and with \( q \) having no zeroes for nonnegative integer arguments. Let \( b \geq 2 \) be an integer, and let \( r_n = p(n)/q(n) \). Then the sequence \( x = (x_0, x_1, x_2, \ldots) \) determined by the iteration \( x_0 = 0 \), and

\[
x_n = \begin{cases} \{bx_{n-1} + r_n\} & \text{if } n > 0 \\
0 & \text{if } n = 0 \end{cases}
\]

(4.5)

either has a finite attractor or is equidistributed in \([0,1)\).

We shall define “equidistributed” and “finite attractor” in Section 4.5. In the meantime we rely on intuition.

**Theorem 4.13.** Assuming Hypothesis 4.0, any constant \( \alpha \) given by a formula of the type \( \alpha = \sum_{k \geq 0} p(k)/(b^k q(k)) \), with \( p(k) \) and \( q(k) \) polynomials as given in Hypothesis 4.0, is either rational or \( b \)-normal.

The proof of this theorem is given in Section 4.5. We should note here that even if a particular instance of Hypothesis 4.0 could be established, it would have significant consequences. For example, if it could be established that the simple iteration given by \( x_0 = 0 \) and

\[
x_n = \left\{2x_{n-1} + \frac{1}{n}\right\}
\]

(4.6)

is equidistributed in \([0,1)\), then it would follow from Theorem 4.0 that \( \log 2 \) is 2-normal. Observe that this sequence is simply the BBP sequence for
log 2. In a similar vein, if it could be established that the iteration given by \(x_0 = 0\) and

\[
x_n = \left\{ 16x_{n-1} + \frac{120n^2 - 89n + 16}{512n^4 - 1024n^3 + 712n^2 - 206n + 21} \right\}
\] (4.7)

is equidistributed in \([0, 1)\), then it would follow that \(\pi\) is 16-normal (and so is 2-normal also). This is the BBP sequence for \(\pi\). The fractional term here is obtained by combining the four fractions in the BBP formula for \(\pi\), namely Equation (3.25), into one fraction, and then shifting the index by one.

Before continuing, we wish to mention a curious phenomenon. Suppose we compute the binary sequence \(y_n = \lfloor 2x_n \rfloor\), where \((x_n)\) is the sequence associated with \(\log 2\) as given in Equation 4.6. In other words, \((y_n)\) is the binary sequence defined as \(y_n = 0\) if \(x_n < 1/2\) and \(y_n = 1\) if \(x_n \geq 1/2\). Theorem 4.0 tells us, in effect, that \((y_n)\) eventually should agree very well with the true sequence of binary digits of \(\log 2\). In explicit computations, we have found that the sequence \((y_n)\) disagrees with 15 of the first 200 binary digits of \(\log 2\), but in only one position over the range 5000 to 8000.

As noted above, the BBP sequence for \(\pi\) is \(x_0 = 0\), and \(x_n\) as given in Equation (4.7). In a similar manner as with \(\log 2\), we can compute the hexadecimal digit sequence \(y_n = \lfloor 16x_n \rfloor\). In other words, we can divide the unit interval into 16 equal subintervals, labeled \((0, 1, 2, 3, \cdots, 15)\), and set \(y_n\) to be the label of the subinterval in which \(x_n\) lies. When this is done, a remarkable phenomenon occurs: The sequence \((y_n)\) appears to perfectly (not just approximately) produce the hexadecimal expansion of \(\pi\). In explicit computations, the first 1,000,000 hexadecimal digits generated by this sequence are identical with the first 1,000,000 hexadecimal digits of \(\pi - 3\). (This is a fairly difficult computation, as it requires roughly \(n^2\) bit-operations, and is not easily performed on a parallel computer system.)

**Conjecture 4.14.** The sequence \(\lfloor 16x_n \rfloor\), where \((x_n)\) is the sequence of iterates defined in equation (4.7), precisely generates the hexadecimal expansion of \(\pi - 3\).

Evidently, this phenomenon arises from the fact that in the sequence associated with \(\pi\), the perturbation term \(r_n = p(n)/q(n)\) is summable, whereas the corresponding expression for \(\log 2\), namely \(1/n\), is not summable. In particular, note that expression (4.4) for \(\alpha = \pi\) gives
\[ ||\alpha_n - x_n|| \leq \sum_{k=n+1}^{\infty} \frac{120k^2 - 89k + 16}{16j^{-n}(512k^4 - 1024k^3 + 712k^2 - 206k + 21)} \]

\[ \approx \frac{120(n+1)^2 - 89(n+1) + 16}{16(512(n+1)^4 - 1024(n+1)^3 + 712(n+1)^2 - 206(n+1) + 21)} \]

so that

\[ \sum_{n=1}^{\infty} ||\alpha_n - x_n|| \leq 0.01579 \ldots \] (4.9)

For the sake of heuristic argument, let us assume for the moment that the \( \alpha_n \) are independent, uniformly distributed random variables in (0, 1), and let \( \delta_n = ||\alpha_n - x_n|| \). Note that an error (i.e. an instance where \( x_n \) lies in a different subinterval of the unit interval than \( \alpha_n \)) can only occur when \( \alpha_n \) is within \( \delta_n \) of one of the points (0, 1/16, 2/16, \ldots, 15/16). Since \( x_n < \alpha_n \) for all \( n \) (where < is interpreted in the wrapped sense when \( x_n \) is slightly less than one), this event has probability 16\( \delta_n \). Then the fact that the sum (4.9) has a finite value implies, by the first Borel-Cantelli lemma, that there can only be finitely many errors [37, pg. 153]. The comparable figure for log 2 is infinite, which implies by the second Borel-Cantelli lemma that discrepancies can be expected to appear indefinitely, but with decreasing frequency. Further, the small value of the sum (4.9) suggests that it is unlikely that any errors will be observed. If instead of summing (4.9) from one to infinity, we instead sum from 1,000,001 to infinity (since we have computationally verified that there are no errors in the first 1,000,000 elements), then we obtain 1.465 \times 10^{-8}, which suggests that it is very unlikely that any errors will ever occur.

### 4.3 A Class of Provably Normal Constants

We now summarize an intriguing recent development in this arena, due to one of the present authors and Richard Crandall, which offers additional hope that the BBP approach may eventually yield the long-sought proof of normality for \( \pi \), \( \log 2 \), and other BBP-type constants [25]. In the previous section, we noted that the 2-normality of

\[ \log 2 = \sum_{n=1}^{\infty} \frac{1}{n2^n} \] (4.10)
4.3. A Class of Provably Normal Constants

rests on the (unproven) conjecture that the iteration given by \( x_0 = 0 \) and \( x_n = \{2x_{n-1} + 1/n\} \) is equidistributed in the unit interval. We now consider the class of constants where the summation defining \( \log 2 \), namely (4.10), is taken over a certain subset of the positive integers:

\[
\alpha_{b,c} = \sum_{n=1}^{\infty} \frac{1}{n^{b/c}} = \sum_{k=1}^{\infty} \frac{1}{c^k \ln^b}, \quad (4.11)
\]

where \( b > 1 \) and \( c > 2 \) are integers. The simplest instance of this class is

\[
\alpha_{2,3} = \sum_{n=3}^{\infty} \frac{1}{n^2} = \sum_{k=1}^{\infty} \frac{1}{3^k 2^k}, \quad (4.12)
\]

\[
= 0.0418836808315029850712528986245716824260967584654857\ldots
\]

\[
= 0.0AB8E38F684BDA12F684BF35BA781948B0FCD6E9E06522C3F35B\ldots.
\]

We first prove the following interesting fact:

**Theorem 4.15.** Each of the constants \( \alpha_{b,c} \), where \( b > 1 \) and \( c > 2 \) are integers, is transcendental.

**Proof.** A famous theorem due to Roth states [174] that if \( |P/Q - \alpha| < 1/Q^{2+\epsilon} \) admits infinitely many rational solutions \( P/Q \) (i.e., if \( \alpha \) is approximable to degree \( 2 + \epsilon \) for some \( \epsilon > 0 \)), then \( \alpha \) is transcendental. We show here that \( \alpha_{b,c} \) is approximable to degree \( c - \delta \). Fix a \( k \) and write

\[
\alpha_{b,c} = \frac{P}{Q} + \sum_{n=k+1}^{\infty} \frac{1}{c^k n^{b/c}}, \quad (4.13)
\]

where \( \gcd(P, Q) = 1 \) and \( Q = c^k b^c \). The sum over \( n \) gives

\[
|\alpha_{b,c} - P/Q| < \frac{2}{c^{k+1} (Q/c^k)^c} < \frac{c^{k c}}{Q^c}. \quad (4.14)
\]

Now \( c^k \log b + k \log c = \log Q \), so that \( c^k < \log Q / \log b \), and we can write

\[
c^{k c} < (\log Q / \log b)^c = Q^{c(\log \log Q - \log \log b) / \log Q}. \quad (4.15)
\]

Thus for any fixed \( \delta > 0 \),

\[
|\alpha_{b,c} - P/Q| < \frac{1}{Q^c (1 + \log \log b / \log \log Q)^c} < \frac{1}{Q^{c-\delta}}, \quad (4.16)
\]

for all sufficiently large \( k \).
Consider now the BBP sequence associated with $\alpha_{2,3}$, namely the sequence defined by $x_0 = 0$, and

$$x_n = \{2x_{n-1} + r_n\}, \quad (4.17)$$

where $r_n = 1/n$ if $n = 3^k$, and $r_n = 0$ otherwise. Successive iterates of this sequence are:

0, 0, 1, 2, 1, 2, 1, 2, 4, 8, 7, 5, 1, 2, 4, 8, 7, 5, 1, 2
13, 26, 25, 23, 19, 11, 22, 17, 7, 14, 1, 2, 4, 8, 16, 5, 10, 20
13, 26, 25, 23, 19, 11, 22, 17, 7, 14, 1, 2, 4, 8, 16, 5, 10, 20
13, 26, 25, 23, 19, 11, 22, 17, 7, 14, 1, 2, 4, 8, 16, 5, 10, 20

A pattern is clear: The sequence consists of a concatenation of triply-repeated segments, each consisting of fractions whose denominators are successively higher powers of 3, and whose numerators range over all integers less than the denominator that are coprime to the denominator. Indeed, the successive numerators in each subsequence are given by the simple linear congruential pseudorandom number generator $z_n = 2z_{n-1} \mod 3^j$ for a fixed $j$.

What we have observed is that the question of the equidistribution of the sequence $(x_n)$ (and, hence, the question of the normality of $\alpha_{2,3}$) reduces to the behavior of a concatenation of normalized pseudorandom sequences of a type (namely linear congruential) that have been studied in mathematical literature, and which in fact are widely implemented for use by scientists and engineers. These observations lead to a rigorous proof of normality for many of these constants. In particular, we obtain the result that each of the constants

$$\alpha_{b,c} = \sum_{n=c^k+1}^{\infty} \frac{1}{nb^n} = \sum_{k=1}^{\infty} \frac{1}{ckb^c}, \quad (4.18)$$

where $b > 1$, and $c$ is co-prime to $b$, is $b$-normal. This result was first given in [25]. We present here a significantly simpler proof, based on the following lemma:
Lemma 4.16. (Hot spot lemma). The constant \( \alpha \) is \( b \)-normal if and only if there exists a constant \( M \) such that for every interval \( (c,d) \),

\[
\limsup_{n \to \infty} \frac{\#0 \leq j < n | \lfloor b^j \alpha \rfloor \in (c,d) |}{n(d-c)} \leq M. \tag{4.19}
\]

This result is proved in [135, pg. 77]. A stronger result is given in [29].

Theorem 4.17. Each of the constants

\[
\alpha_{b,c} = \sum_{k=1}^{\infty} \frac{1}{c^k b^{e^k}}, \tag{4.20}
\]

where \( b > 1 \), and \( c \) is co-prime to \( b \), is \( b \)-normal.

Proof. For convenience, we will establish the result for \( \alpha = \alpha_{2,3} \). Let \( (x_n) \) be the BBP sequence associated with \( \alpha \), as given in (4.17). From this pattern it follows that if \( n < 3^p + 1 \) then \( x_n \) is a multiple of \( 1/3^p \). Also, it follows by the proof of Theorem 4.11, that

\[
|x_n - \{2^n \alpha\}| = \left| \sum_{k=n+1}^{\infty} 2^{n-k} r_k \right| < \frac{1}{2n}. \tag{4.21}
\]

Suppose we are given some half-open interval \( [c,d) \). Observe, in view of (4.21), that if \( \{2^j \alpha\} \in [c,d) \), then \( x_j \in [c-1/(2j), d+1/(2j)) \). Let \( n \) be any integer greater than \( 1/(d-c)^2 \), and let \( 3^p \) denote the largest power of 3 less than or equal to \( n \), so that \( 3^p \leq n < 3^{p+1} \). Let \( m = \lceil 1/(d-c) \rceil + 1 \). Now note that for \( j \geq m \), we have \( [c-1/(2j), d+1/(2j)) \subset [c - (d-c)/2, d + (d-c)/2) \). Since the length of this latter interval is \( 2(d-c) \), the number of multiples of \( 1/3^p \) that it contains is either \( \lfloor 2 \cdot 3^p (d-c) \rfloor \) or \( \lfloor 2 \cdot 3^p (d-c) \rfloor + 1 \). Thus there can be at most three times this many \( j \)'s less than \( n \) for which \( x_j \in [c - (d-c)/2, d + (d-c)/2) \). Therefore we can write

\[
\frac{\#0 \leq j < n | \lfloor 2^j \alpha \rfloor \in [c,d) |}{n(d-c)} \leq \frac{m + \#m \leq j < n (x_j \in [c - (d-c)/2, d + (d+c)/2))}{n(d-c)} \leq \frac{m + 3(2 \cdot 3^p (d-c) + 1)}{n(d-c)} < 8.
\]

We have shown that for all \( d-c \),

\[
\limsup_{n \geq 1} \frac{\#0 \leq j < n | \lfloor 2^j \alpha \rfloor \in [c,d) |}{n} \leq 8(d-c),
\]
so by the hot spot theorem, \( \alpha \) is 2-normal.

We should add that \( \alpha_{2,3} \) was actually proven 2-normal by Stoneham in 1970 [184]. The new BBP-based approach described above now makes it possible to extend these and other previous results to a much larger class. For example, it is shown in [25] that all constants of the form

\[
\alpha_{2,3}(r) = \sum_{k=1}^{\infty} \frac{1}{3^k2^{3^{r_k}+r_k}},
\]

(4.22)

where \( r_k \) is the \( k \)-th bit in the binary expansion of \( r \in (0, 1) \), are 2-normal and transcendental. It is easily to show that if \( r \neq s \), then \( \alpha_{2,3}(r) \neq \alpha_{2,3}(s) \). In other words, for every real number \( r \in (0, 1) \), there corresponds a distinct real constant \( \alpha_{2,3}(r) \). Since there are uncountably many reals in \( (0, 1) \), it follows that there are uncountably many 2-normal, transcendental numbers of the form given by (4.22).

As an amusing sideline, these \( \alpha \) constants also possess the rapid individual digit computation property possessed by conventional BBP-type constants. Furthermore, in this case the computation is extraordinarily rapid. For example, the googol-th (i.e., the \( 10^{100} \)-th) binary digit of \( \alpha_{2,3} \) can be calculated in less than one second on a 2003-era computer. The digit is 0. The first ten hexadecimal digits starting at this position are 2205896E7B.

### 4.4 Algebraic Irrationals

Although there is no proof of this assertion, as far as we can tell, there are no BBP-type formulas for algebraic irrationals such as \( \sqrt{2}, \sqrt{10} \) and \( \phi = (1+\sqrt{5})/2 \). Thus it appears that the theory we have developed above to address the question of normality for BBP-type constants is inapplicable to the case of algebraic irrationals. Yet from all available experimental evidence, these constants are also \( b \)-normal for all commonly used number bases. In any event, even basic questions such as whether the decimal expansion of \( \sqrt{2} \) has infinitely many fives remain unanswered.

Recently, some results on the density of ones in binary expansions of certain algebraic irrationals were obtained by the present authors, Richard Crandall, and Carl Pomerance [19]. These results are certainly much weaker than full normality, but are worth mentioning given the paucity of results in this arena.
If $a$ is an integer, we shall define $B(a)$ as the number of ones in the binary representation of $a$. If $x$ is real, $0 < x < 1$, then by $B_n(x)$, we shall mean the number of ones in the first $n$ binary digits of $x$ after the “decimal” point. Note that if $x$ is a binary fraction (i.e., $x = c/2^d$ for integers $c$ and $d$), then $x$ has two valid binary expansions—one terminating in zeroes and the other terminating in ones. Thus in such instances below, we shall clarify which expansion we mean. For a rational number $r$ with $0 < r < 1$, we define the function $C(r) = 1$ in the case that $r$ is a binary fraction; otherwise, $C(r) = c/d$, where $c$ is the number of ones in the terminally repeating block of digits in the binary expansion of $r$, and where $d$ is the length of the block of repeating digits.

For real numbers $x$ and $y$, with $0 < x < 1$ and $0 < y < 1$, we use the notation $(A_k(x, y, n), 0 \leq k < 2^n)$ to denote the acyclic convolution of the first $n$ binary digits of $x$ and the first $n$ binary digits of $y$. To be specific, let the binary digits of $x$ and $y$ be indexed starting with 0. Then

$$A_k(x, y, n) = \sum_{j=0}^{n-1} x_j y_{k-j}, \quad 0 \leq k < 2^n,$$

where by the subscript $k - j$ we mean $k - j + n$ if $k < j$.

**Theorem 4.18.** Let $r$ be a rational number, $0 < r < 1$, and suppose that $s = \sqrt{r}$ is irrational. Then

$$\liminf_{n \to \infty} \frac{B_n(s)}{\sqrt{C(r)n}} \geq 1,$$

We first prove two lemmas.

**Lemma 4.19.** For any two positive integers $a$ and $b$, $B(a + b) \leq B(a) + B(b)$, and $B(ab) \leq B(a)B(b)$. The same is true for reals, namely $B_n(x + y) \leq B_n(x) + B_n(y)$ and $B_n(xy) \leq B_n(x)B_n(y)$, provided we first trim $x$ and $y$ to $n$ bits.

**Proof.** The assertion on sums is easily shown by verifying it for one- and two-bit values of $a$ and $b$, and then arguing by induction on the number of bits in $a$ and $b$. The assertion on products follows from the first by observing that the process of binary multiplication is merely a sequence of binary additions with shifts by appending zeroes. \qed
For $x$ and $y$ with $0 < x, y < 1$, define
\[
z_n(x, y) = \sum_{k=0}^{2n-1} A_k(x, y, n) 2^{-k-1}.
\] (4.23)

Then $|z_n(x, y) - xy| < 2^{1-n}$. In other words, the binary expansion of $z_n(x, y)$ agrees with $x \cdot y$ up to approximately $n$ digits (it might be slightly fewer because of trailing ones, but the bound still holds).

**Proof.** This follows by the simple observation that the acyclic convolution reproduces the process of multiplication of two binary fractions. The error in using only the first $n$ bits of the two operands can be found as follows. Write $x = \alpha_n + \beta_n$, where $\alpha_n$ is the value obtained by using only the first $n$ bits of the binary expansion of $x$, with $\beta < 2^{-n}$, and similarly write $y = \gamma_n + \delta_n$. Since $z_n(x, y) = \alpha_n \gamma_n$ precisely, we have
\[
|z_n(x, y) - xy| < \alpha_n \delta_n + \gamma_n \beta_n + \beta_n \delta_n < 2 \cdot 2^{-n} = 2^{1-n}. \tag{4.24}
\]

Note that $z_n(x, y)$ is always an underestimate of $xy$, except in the case where $x$ and $y$ are binary fractions represented using the expansion terminating in zeroes, in which case $z_n(x, y) = xy$ exactly for all sufficiently large $n$.

**Proof of Theorem 4.0.** In the hypothesis of Theorem 4.0, $r$ is rational, but $s = \sqrt{r}$ is irrational. Since $s$ is irrational, $|z_n(s, s) - r| < 2^{1-n}$, and further since the binary expansion of $s$ has infinitely many ones (and it cannot terminate in zeroes or ones), $z_n(s, s)$ will always underestimate $s^2 = r$. In the case that $r$ is a binary fraction, this underestimation means that the approximations $z_n(s, s)$ cannot possibly replicate the binary expansion that terminates in zeroes, but they can and therefore must replicate with increasing fidelity the expansion that terminates in ones. In the case that $r$ is not a binary fraction, the approximations $z_n(s, s)$ must replicate with increasing fidelity the unique binary expansion of $r$. Here by “replicate with increasing fidelity,” we mean that the relevant binary expansions of $z_n(s, s)$ and $r$ agree for all digits up to some position $n - d$ for some fixed integer $d$.

Here we observe that Lemma 4.0 also applies to the real fraction multiplication (i.e., convolution) process described in Lemma 4.0. Thus $B_n(z_n(s, s)) \leq B^2_n(s)$. Now since $z_n(s, s)$ replicates with increasing fidelity the expansion of $r$, we must have, at the least,
\[
\liminf_{n \to \infty} \frac{B_n(z_n(s, s))}{n} = \liminf_{n \to \infty} \frac{B_n(r)}{n}. \tag{4.25}
\]
4.5. Periodic Attractors and Normality

But since $B_n(r)/n$ converges to $C(r)$, this means that given $\epsilon > 0$,

$$n(B_n(s)/n)^2 \geq B_n(z_n(s,s))/n \geq B_n(r)/n - \epsilon \geq C(r) - 2\epsilon$$  \hspace{1cm} (4.26)

for all sufficiently large $n$, which establishes our result. \hfill \Box

Theorem 4.0 only applies to irrational square roots of rational numbers. In a new paper (2003) by the present authors, Richard Crandall, and Carl Pomerance, this result has been significantly strengthened to the following:

**Theorem 4.21.** For positive real algebraic $x$ of degree $d > 1$ and for any $\epsilon > 0$ there exists some $N$ (depending on $x$ and $\epsilon$) such that for all $n > N$,

$$B_n(x) > (1 - \epsilon)(2a_d)^{-1/d}n^{1/d},$$

where $a_d > 0$ is the leading coefficient of the minimum integer polynomial for $y = x/2^\lfloor \log_2 x \rfloor$.

The proof of this result is given in [19]. Interestingly, this proof involves “BBP tails,” or, in other words, BBP sums beyond certain digit positions, driving home once more the usefulness of the BBP idea.

 Whereas with Theorem 4.0, we had that the number of ones in the first $n$ bits of an irrational square root is asymptotically at least a constant times $\sqrt{n}$, with Theorem 4.0 we have a constant times the $d$-th root of $n$, where $d$ is the algebraic degree. So, for example, the number of ones in the first $n$ bits of $\sqrt[3]{2}$ must be at least some constant times $\sqrt[3]{n}$. Obviously we do not believe that this is the strongest result possible. All experimental evidence suggests that the limiting density of ones in the binary expansion of any algebraic irrational is not only greater than zero, but in fact is precisely $1/2$, and further that the density of each of the four two-bit combinations is $1/4$, etc. But lacking formal proof, such a supposition could conceivably be incorrect.

4.5 Periodic Attractors and Normality

In this section, we shall prove the result mentioned above, namely Theorem 4.0, which implies normality for irrational BBP-type constants, conditional on Hypothesis 4.0. For some additional results and full details, consult [24], from which we have adapted this material. First, some preliminaries:

As before, we define the norm $||\alpha||$ for $\alpha \in [0,1]$ as $||\alpha|| = \min(\alpha, 1 - \alpha)$. With this definition, $||\alpha - \beta||$ measures the shortest distance between $\alpha$ and
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$\beta$ on the unit circumference circle in the natural way. A simple result, which we will term the “dilated-norm rule,” is the following: If $0 \leq \delta \leq 1/(2||z||)$, then because $||\delta z||$ is now bounded above by $1/2$, we have $||\delta z|| = \delta||z||$.

A base-$b$ expansion $\alpha = 0.\alpha_1\alpha_2\alpha_3 \cdots$, where each $\alpha_j$ is an integer in $[0, b-1]$, is taken to be unique for $\alpha$. When competing expansions exist, as in decimal $0.1000\ldots = 0.0999\ldots$, we select the variant with trailing zeroes.

We define the frequency (when it exists) with which a given finite digit string $(d_1 d_2 \cdots d_k)$ appears in $\alpha$ to be the limit as $N \to \infty$ of the number of instances where $\alpha_j = d_1$, $\alpha_{j+1} = d_2$, $\cdots$, $\alpha_{j+k-1} = d_k$, $j \leq N + 1 - k$, divided by $N$.

For a sequence $x = (x_0, x_1, \cdots)$ of real numbers in $[0, 1)$, we define the counting function

$$C(x, c, d, N) = \#(x_j \in [c, d) : j < N).$$

In other words, the $C$ function gives the count of the first $N$ elements of the sequence $x$ that lie in the interval $[c, d)$. We now introduce a standard definition from the literature:

**Definition 4.22.** A sequence $x$ in $[0, 1)$ is said to be equidistributed if for any $0 \leq c < d < 1$ we have

$$\lim_{N \to \infty} \frac{C(x, c, d, N)}{N} = d - c.$$ 

This definition is identical to that of “uniform distribution modulo 1,” as given in [135] p.1. The following two basic results are taken from that source:

**Theorem 4.23.** Let $(x_n)$ be equidistributed. If a sequence $(y_n)$ has the property that $\{y_n\} \to \beta$ (constant $\beta$) as $n \to \infty$, then the sequence $\{(x_n + y_n)\}$ is likewise equidistributed. In particular, if $y_n \to 0$, then $\{(x_n + y_n)\}$ is equidistributed.

**Theorem 4.24.** A number $\alpha$ is $b$-normal if and only if the sequence $(\{b^n\alpha\} : n = 1, 2, 3, \cdots)$ is equidistributed.

We now define the notions of finite attractor and periodic attractor:

**Definition 4.25.** A sequence $x = (x_n)$ in $[0, 1)$ is said to have a finite attractor $W = (w_0, w_1, \cdots, w_{P-1})$ if for any $\epsilon > 0$, there is some $K = K(\epsilon)$ such that for all $k \geq 0$, we have $||x_{K+k} - w_{t(k)}|| < \epsilon$, for some function $t(k)$, with $0 \leq t(k) < P$. 
4.5. Periodic Attractors and Normality

Definition 4.26. A sequence \( x = (x_n) \) in \([0, 1)\) is said to have a periodic attractor \( W = (w_0, w_1, \cdots, w_{P-1}) \), if for any \( \epsilon > 0 \), there is some \( K = K(\epsilon) \) such that for any \( k \geq 0 \), we have \( ||x_{K+k} - w_k \mod P|| < \epsilon \).

Theorem 4.27. Assume a sequence \( (y_n) \) has the property that \( y_n \to \beta \) (with \( \beta \) constant) as \( n \to \infty \). Then a sequence \( (x_n) \) in \([0, 1)\) has a finite attractor (alternatively, a periodic attractor) if and only if \( \{x_n + y_n\} \) does.

Proof. This follows immediately from the \( \epsilon \)-restriction in the definitions of finite attractor and periodic attractor. \( \square \)

We will now show that in certain cases of interest here, these two notions of attractor coincide:

Theorem 4.28. Let \( \alpha \) be real and assume an integer base \( b \geq 2 \). If the sequence \( x = (b^i\alpha) \) has a finite attractor \( W \), then \( W \) is a periodic attractor, and the structure of the attractor \( W \) is necessarily

\[
W = (w_0, \{bw_0\}, \{b^2w_0\}, \cdots, \{b^{P-1}w_0\}).
\]

Moreover, each element in \( W \) is rational.

Proof. Let \( W = \{w_0, w_1, \cdots, w_{P-1}\} \) be the finite attractor for \( x \). Let \( d = \min_{0 \leq i < P} ||w_i - w_j|| \), and choose \( \epsilon < d/(4b) \). Let \( W' \) be the set of all \( z \) in \([0, 1)\) such that \( ||z - w_i|| < \epsilon \) for some \( 0 \leq i < P \). Then we know that there is some \( K'(\epsilon) \) such that for all \( k > K' \) we have \( x_k \in W' \). Let \( K \) be the first \( k > K' \), such that \( ||x_k - w_0|| < \epsilon \). We then have:

\[
||x_{K+1} - bw_0|| = ||bx_K - bw_0|| = b||x_K - w_0|| < b\epsilon < d/4, \tag{4.27}
\]

where the second equality follows from the bounded dilation rule mentioned at the start of the present section.

It follows that \( x_{K+1} \) is within \( \epsilon \) of \( \{bw_0\} \), and similarly \( x_{K+k+1} \) is within \( \epsilon \) of \( \{bw_k\} \) whenever \( x_{K+k} \) is within \( \epsilon \) of \( w_0 \), which must occur infinitely often. Since there can be at most one element of the attractor set \( W \) in the region of size \( d/4 \) about \( \{bw_0\} \), and since the choice of \( \epsilon \) above was arbitrary, we conclude that \( bw_0 \) must be the element of \( W \) in that region. We can for notational convenience assume that \( w_1 = \{bw_0\} \). Then \( ||x_{K+1} - w_1|| < \epsilon \), and the argument can be repeated to show that \( x_{K+2} \) is close to \( w_2 = \{b^2w_0\} \), etc., and finally that \( x_{K+P-1} \) is close to \( w_{P-1} = \{b^{P-1}w_0\} \). It then follows that the member of \( W \) which \( x_{K+P} \) is close to must be \( w_0 \), since otherwise the \( \epsilon \) region around \( w_0 \) would never be visited again by the \( x \) sequence and thus \( w_0 \) could not be a member of...
4. Normality of Numbers

the attractor set. Therefore, \( W = (w_0, \{b w_0\}, \ldots, \{b^{P-1} w_0\}) \), and \( W \) is a periodic attractor for the \( x \) sequence. Rationality of the attractor points is demonstrated by noting the periodicity condition \( w_0 = \{b^P w_0\} \), which implies that for some integer \( m \), we have \( w_0 = m/(b^P - 1) \), and similarly for the other \( w_i \in W \).

**Theorem 4.29.** *If the sequence \((x_n)\) as defined by \( x_0 = 0, x_n = \{bx_{n-1} + r_n\} \), where \( b \) is a positive integer, \( r_n \to 0 \) and \( r_n \neq 0 \), has a finite attractor \( W \), then \( W \) is a periodic attractor, and each element of \( W \) is rational.*

**Proof.** Let \( W = \{w_0, w_1, \ldots, w_{P-1}\} \) be the finite attractor for \( x \). Let \( d = \min_{0 \leq i, j < P} (||w_i - w_j||) \), and choose \( \epsilon < d/(4b + 4) \). Let \( W_\epsilon \) be the set of all \( z \) in \([0, 1)\) such that \( ||z - w_i|| < \epsilon \) for some \( 0 \leq i < P \). Then we know that there is some \( K'(\epsilon) \) such that for all \( k > K' \), we have \( x_k \in W_\epsilon \) and \( |r_k| < \epsilon \). Let \( K \) be the first \( k > K' \), such that \( ||x_k - w_0|| < \epsilon \). We then have (again we use the dilated-norm rule from the start of the present section):

\[
||x_{K+1} - bw_0|| = ||bx_K + r_{K+1} - bw_0|| \leq b||x_K - w_0|| + \epsilon < (b + 1)\epsilon < d/4.
\]  

(4.28)

The remainder of the proof of this result follows the second paragraph of the proof of Theorem 4.0. \( \square \)

Now we are in a position to establish the following result:

**Theorem 4.30.** *The sequence \( \{b^n \alpha\} \) has a finite attractor if and only if \( \alpha \) is rational.*

**Proof.** Assume that the sequence \( \{b^n \alpha\} \) has a finite attractor. By Theorem 4.0 it then has a periodic attractor. In the definition of a periodic attractor, let \( K \) be the index corresponding to \( \epsilon = 1/(4b) \), and set \( h = ||x_K - w_0|| \). Suppose \( h > 0 \). Then let \( m = \lfloor \log_h(\epsilon/h) \rfloor \), and note that \( b^m h \leq \epsilon < b^{m+1}h < be < 1/4 \). Thus we can write (once again using the dilated-norm rule):

\[
||x_{K+m+1} - w_{m+1} \mod p|| = ||b^{m+1}x_K - b^{m+1}w_0|| = b^{m+1}||x_K - w_0|| = b^{m+1}h > \epsilon.
\]  

(4.29)

But this contradicts the definition of the periodic attractor. Thus we conclude that \( h = 0 \), so that \( x_{K+k} = w_k \mod p \) for all \( k \geq 0 \). In other words, after at most \( K \) initial digits, the base-\( b \) expansion of \( \alpha \) repeats with period \( P \), so that \( \alpha \) is rational. As for the converse, \( \alpha = p/q \) rational implies
the sequence \((b^n p/q) = ((p b^n) \mod q)/q)\) is periodic, having in fact the period 1 for \(\alpha = 0\) and, for \(p/q\) in lowest terms, the period of the powers of \(b\) modulo \(q\).

We may now prove Theorem 4.0.

**Theorem 4.0.** Assuming Hypothesis 4.0, every irrational constant with a BBP-type formula for a given base \(b\) is \(b\)-normal.

**Proof.** Assume Hypothesis 4.0. Then suppose a real number \(\alpha\) possesses a formula of the form

\[
\alpha = \sum_{k=1}^{\infty} \frac{p(k)}{b^k q(k)},
\]

where \(p(k)\) and \(q(k)\) are integer polynomials, with \(\deg p < \deg q\) and with \(q(k)\) not having any zeroes for positive integers \(k\). We first observe that \(\alpha\) is rational if and only if the sequence \((x_n)\), where

\[
x_n = \left\{b x_{n-1} + \frac{p(n)}{q(n)}\right\}
\]

has a finite attractor. To see this, we know from Theorem 4.0 that the sequence \(\{b^n \alpha\}\) has a periodic attractor if and only if \(\alpha\) is rational. Following the BBP strategy, we can write

\[
\{b^n \alpha\} = \left\{\sum_{k=1}^{n} \frac{b^{n-k} p(k)}{q(k)} + \sum_{k=n+1}^{\infty} \frac{b^{n-k} p(k)}{q(k)}\right\} = \{x_n + t_n\},
\]

where \(x\) is defined by \(x_0 = 0\) and the recursion

\[
x_n = b x_{n-1} + \frac{p(n)}{q(n)}
\]

with the sequence \(t\) given by

\[
t_n = \sum_{k=1}^{\infty} \frac{1}{b^k q(k+n)}.
\]

Provided that \(\deg p < \deg q\) as in Hypothesis 4.0, given any \(\epsilon\) there is some \(n\) such that \(|p(k+n)/q(k+n)| < \epsilon\) for all \(k \geq 1\). For such \(n\), we have \(|t_n| < \epsilon \sum_{k \geq 1} b^{-k} = \epsilon/(b - 1) < \epsilon\). Thus \(t_n\) converges to zero as \(n \to \infty\). Hence, it follows from Theorem 4.0 that \((x_n)\) has a periodic attractor if and only if \(\alpha\) is rational.
4.6 Commentary and Additional Examples

1. **Borel’s normal number theorem.** This theorem asserts that almost every real number has normally distributed digits in any or all bases. It is a special case of the strong law of large numbers applied to Bernoulli trials, or of the first Borel-Cantelli lemma that if a sequence of events $A_n$ is such that $\sum_n P(A_n)$ converges, then $\lim \sup_n A_n = \bigcup_n \bigcap_{m>n} A_m = 0$.

(a) Show that the real numbers in $I = [0,1]$ with no fives in prime positions base ten form a negligible set.

(b) Prove the Borel normal law for binary numbers. **Hint:** Let $s_n(\omega) = \sum_{k=1}^{n} r_k(\omega)$ where

$$r_k(\omega) = \begin{cases} +1, & d_k = 1 \\ -1, & d_k = 0, \end{cases}$$

and $d_k = d_k(\omega)$ is the $k$-th digit of $\omega$. Note that $s_n(\omega)/n \to 0$ if and only if $\sum_{k\leq n} d_k(\omega)/n \to 1/2$. Show for $\varepsilon > 0$ that

$$P[\omega : |s_n(\omega)| \geq n\varepsilon] \leq \frac{1}{n^4 \varepsilon^4} \int_0^1 s_n^4 d\omega.$$  

Then show that

$$\int_0^1 s_n^4 d\omega = n + 3n(n-1)$$

and deduce the $P[\omega : |s_n(\omega)| \geq n\varepsilon] \leq 3/(n^2 \varepsilon^4)$. If we choose $\varepsilon_n$ appropriately $\sum_n P[\omega : |s_n(\omega)| \geq n\varepsilon_n]$ is finite. Conclude that $s_n(\omega)/n \to 0$ for almost all $\omega$ and observe that this is the asserted conclusion.

(c) Generalize this to an arbitrary base. Conclude that almost every number is absolutely normal. In 1916, Sierpinski gave an “effective” construction of an absolutely normal number. This has recently been expressed recursively in [32]. There are still no “natural” examples of absolutely normal numbers, unless one considers Chaitin’s constant to be one.

The second Borel-Cantelli lemma shows that for a sequence of independent events when $\sum_n P(A_n)$ diverges, then $\lim \sup_n A_n = 1$. Together they provide a “zero-one” law. Full details are in [37].
2. **The normal numbers are small topologically.** We note that while the absolutely normal numbers comprise a set of full measure, Salt proved in 1966 that it is of the first Baire category. Indeed, let \( b, r, \) and \( n \) be integers \( 0 \leq r < b, \ b > 1, \) and for \( 0 \leq x < 1, \) let \( N_n(r, x) \) denote the number of occurrences of \( r \) in the first \( n \) terms of the base-\( b \) expansion of \( x, \) and let \( L(r, x) \) denote the set of limit points of the sequence whose \( n \)th term is \( N(r, x)/n. \) Then \( L(r, x) = [0, 1] \) for all \( x \in [0, 1) \) with the exception of a set of the first category (i.e., a countable union of nowhere dense sets). By contrast, the Liouville numbers form a set of transcendental numbers of measure zero whose complement is first category \([49] \) pg. 352).

3. **Rational times normal is normal.**

**Theorem 4.31.** Whenever \( \alpha \) is normal to base \( b, \) then so is \( r\alpha \) for every nonzero positive rational \( r. \)

**Proof.** This result is an example application of the hot spot lemma, namely Lemma 4.0. First, suppose that \( \alpha \) is normal, and consider \( p\alpha \) for a positive integer \( p. \) Let \( \{\cdot\} \) denote fractional part. Then \( \{b^j\alpha\} \in [x, y) \) implies that one of the following \( p \) mutually exclusive conditions must hold:

\[
\begin{align*}
\{b^j\alpha\} &\in [x/p, y/p) \\
\{b^j\alpha\} &\in [x/p+1/p, y/p+1/p) \\
\{b^j\alpha\} &\in [x/p+2/p, y/p+2/p) \\
\vdots & \\
\{b^j\alpha\} &\in [x/p+(p-1)/p, y/p+(p-1)/p).
\end{align*}
\]

Since \( \alpha \) is normal, the limiting frequency of each of the above is \((y-x)/p. \) Thus the limiting frequency of \( \{b^j\alpha\} \in [x, y) \) is \( p \) times this value, or \( y-x. \) This establishes that \( p\alpha \) is normal.

Now suppose that \( \alpha \) is normal, and consider \( \alpha/p \) for a positive integer \( p. \) We can assume that \( y-x < 1/p, \) because otherwise we can take \( C = 2p \) in the condition of Theorem 4.0. Then \( \{b^j\alpha/p\} \in [x, y) \) implies \( \{b^j\alpha\} \in \{(px), (py)\}, \) where we understand that in some cases \( \{px\} > \{py\}, \) due to “wrapping” around the unit interval, in which case we take this to mean the union of the two intervals \([0, \{py\}) \) and \( [(px), 1). \) However, in either case, the total length is \( p(y-x), \) so that the limiting frequency of \( \{b^j\alpha\} \) in this set is \( p(y-x). \) Thus we can
write
\[
\limsup_{n \to \infty} \frac{\#0 \leq j \leq n-1 \{b^j \alpha/p \in [x, \gamma]\}}{n} \leq p(\gamma - x),
\]
where we must use \( \leq \) since whereas \( \{b^j \alpha/p \in [x, \gamma]\} \) implies \( \{b^j \alpha \in [(px, py]\} \), the converse is not true. But this is good enough for Theorem 4.0 which then implies that \( \alpha/p \) is normal. This proof is taken from [28]. See also exercise 8.9 in [135] pg. 77. 

4. Rational plus normal is normal.

**Theorem 4.32.** Whenever \( \alpha \) is normal to base \( b \), then so is \( r + \alpha \) for every nonzero positive rational \( r \).

**Proof.** This proof is left as an exercise (see proof of Theorem 4.0 above).

5. **Proof that Champernowne’s constant is 10-normal.** Using the hot spot lemma, one can fairly easily prove that Champernowne’s number \( C = 0.12345678910111213141516 \ldots \) is 10-normal:

(a) Observe that the decimal expansion of \( C \) consists of a concatenation of sections of \( k \)-long integers, with section \( k \) having length \( L_k = 9k10^{k-1} \).

(b) Within section \( k \), observe, by experimental calculations if desired, that among all \( j \)-long strings of decimal digits with \( j \leq k \), the all-ones string appears most frequently, and this string appears \( A_{j,k} = (j + 9k)10^{k-j-1} \) times. Prove that this expression (or a somewhat larger upper bound) holds. *Hint:* Enumerate the number of ways a \( j \)-long string of ones is entirely contained within a \( k \)-digit integer, and also the number of instances where a \( j \)-long string of ones spills from one \( k \)-digit integer to the next, in the Champernowne expansion.

(c) Let \( n_k \) denote the positions of the successive ends of sections in the Champernowne expansion, i.e., \( n_k = L_1 + L_2 + \cdots + L_k \). Calculate an upper bound for \( c_{j,k} = A_{j,1} + A_{j,2} + \cdots + A_{j,k} \), the total count of appearances of the \( j \)-long all-one string through the end of section \( k \).

(d) Apply the hot spot lemma, namely Lemma 4.0 to prove that \( C \) is 10-normal. *Hint:* Note that for \( n_{k-1} < n < n_k \), the count
of appearances of any \( j \)-long string in the first \( n \) digits is no greater than \( c_{j,k} \), and that for \( n \) in this range, \( n > L_{k-1} \). Also observe that any given interval contains a subinterval with decimal fraction endpoints, with length at least \( 1/10 \) of the length of the interval.

6. Density of binary digits in algebraic irrationals. In some analysis of the density of binary digits in the expansions of certain algebraic irrationals, the present authors, together with Richard Crandall and Carl Pomerance, attempted to estimate the following function, as \( R \) goes to infinity:

\[
U_d(R) = \sum_{m=1}^{\infty} \frac{(R+m+d-1)}{2^m} \quad (r, D \in \mathbb{N}).
\]

(a) It is easy to discover that \( U_d(R) \) satisfies the recursion

\[
f(R, d) - 2 f(R, d - 1) = \binom{R + d - 1}{d - 1}.
\]

(4.33)

Now Maple can “tell” one that

\[
U_d(R) = \frac{1}{2} \left( \binom{R + d}{d - 1} \right) F \left( 1, d + R + 1, R + 2; \frac{1}{2} \right),
\]

(4.34)

and a computer-algebra-assisted use of Euler’s integral for the hypergeometric function simplifies to

\[
\sum_{m=1}^{\infty} \frac{(R+m+d-1)}{2^m} = \int_1^1 (2-x)^{d-1} x^R \, dx \frac{\beta(R+1, d)}{\beta(R+1, d)} (4.35)
\]

(the \( \beta \) function is discussed in Section 5.4). From (4.35), it is fairly easy to obtain precise asymptotics and estimates as needed. However, it is more relevant that it is now easy by computer to show that the right side of (4.35), call this \( V_d(R) \), satisfies (4.33). As

\[
V_1(R) = (R + 1) \int_0^1 x^R \, dx = \sum_{m=1}^{\infty} \frac{1}{2^m} = U_1(R) = 1,
\]

we are done, in what is an exemplary use of experimental math.

(b) Problem. Compute a good upper bound for \( U_d(R) \) for large \( R \) and determine its asymptotic behaviour in \( R \).
Answer. We assume \( R > d \) and begin by writing

\[
\mathcal{K}(R, d) = \int_0^1 (2 - x)^{d-1} x^R \, dx,
\]  

so that

\[
V_d(R) = \frac{\mathcal{K}(R, d)}{\beta(R + 1, d)}. 
\]  

Observe with a change of variables

\[
\frac{1}{R+1} < \mathcal{K}(R, d) = \int_0^1 (1 + t)^{d-1} (1 - t)^R \, dt
\]

\[
= \int_0^1 (1 - t^2)^{d-1} (1 - t)^{R+1-d} \, dt
\]

\[
< \int_0^1 (1 - t)^{R+1-d} \, dt = \frac{1}{R + 2 - d},
\]

where the lower bound comes from estimating the original integral. In a similar manner,

\[
\frac{1}{\beta(R + 1, d)} = \frac{\Gamma(R + 1 + d)}{\Gamma(R + 1) \Gamma(d)} = \frac{1}{(d-1)!} \prod_{k=1}^d \left(1 + \frac{k}{R}\right)
\]

\[
< \frac{R^d}{(d-1)!} \left(1 + \frac{d}{R}\right)^d < \frac{R^d}{(d-1)!} e^{d/R}.
\]

Combining these last two inequalities yields

\[
U_d(R) < \left[\frac{R}{R + 2 - d} \, e^{d/R}\right] \frac{R^{(d-1)}}{(d-1)!},
\]

for \( R > d \). If we call this last bracketed expression \( \gamma_d(R) \), we see that

\[
\frac{R}{R + 2} \leq \gamma_d(R) < \left(1 + \frac{1}{m}\right) e^{\frac{d}{mR}}
\]

for \( R > m d, m \geq 1 \). Thus, globally the constant is bounded above by \( 2 \sqrt{e} \) and asymptotically in \( R \) the upper and lower bounds tend to 1. This also shows

\[
\limsup_{R \to \infty} \frac{U_d(R)}{(R^{(d-1)}/(d-1)!)} \leq 1.
\]
We leave it to the reader to show, using Stirling’s formula, that indeed
\[
\lim_{R \to \infty} \frac{U_d(R)}{(R^{d-1}/(d-1)!)} = 1.
\]

(c) Show that
\[
U_d(R) = \sum_{j=0}^{d-1} \binom{R + d}{j}.
\]

See [19] for further details.

7. **Sierpinski’s number.** As noted in this chapter, in 1916 Sierpinski gave an “effective” construction of an absolutely normal number, \(\sigma\), recently expressed recursively in [32]. That said, the present algorithm does not allow computation of any digits of \(\sigma\). It would be very interesting to rectify this state of affairs.

8. **A normal number as a pseudorandom number generator.**

Recall the constant \(\alpha_{2,3}\) defined in Section 4.3, which is known to be 2-normal. The binary expansion of \(\alpha_{2,3}\) is a good pseudorandom bit generator, and the sequence \(y_n = \{2^n \alpha_{2,3}\}\) of shifted fractional parts is a good \((0,1)\) uniform pseudorandom number generator. In particular, the sequence \(y_{53n}\) can be used to generate independent 64-bit IEEE floating-point iterates, each with 53 bits of \(\alpha_{2,3}\), with a scheme that can be easily implemented in any programming language and is well suited for parallel computation:

(a) Observe that in the sequence (4.17), each section of length \(2 \cdot 3^k\) starts with \(\lfloor 3^k/2 \rfloor / 3^k\).

(b) Note that if \(m\) is the largest power of three less than \(n\), then
\[
x_n = \frac{2^n - m \lfloor m/2 \rfloor \mod m}{m}.
\]

The exponentiation here can be done using Algorithm 3.0 (Section 3.4), implemented using 128-bit integer or double-double floating-point arithmetic (see Section 6.2.1).

(c) Observe that if \(y_n\) is the sequence of shifted fractional parts as defined above, then \(x_n\) is identical to \(y_n\), to within the 53-bit accuracy of IEEE double floating-point arithmetic, provided that \(n\) is not within 100 of a power of three. *Hint:* Recall the proof of Theorem 4.0.
(d) Observe that the numerators of successive elements of the sequence \( x_{53n} \) (within a \( 2m/3 \)-long segment) can be generated using the iteration \( x_{53(n+1)} = qx_{53n} \mod m \), where \( q = 2^{53} \).

(e) Implement this scheme on a computer, generating \( n \) independent IEEE 64-bit floating-point values in \((0, 1)\), each with successive 53-bit sections of \( \alpha_{2,3} \), beginning at a given starting index \( a \) in the binary expansion of \( \alpha_{2,3} \), subject to the assumed restriction that the range \( a \leq j < a + n \) does not include any value within 100 of a power of 3.

(f) Show that the period of the resulting pseudorandom number generator is \( 2m/3 \), where \( m \) is the largest power of three less than or equal to the starting index \( a \). \( \text{Hint: See [130]} \text{ pg. 21].} \)
What range should \( a \) be chosen in, so as to insure that the period is as large as possible, yet not so large as to result in numeric overflows, given the computer arithmetic being used (say 128-bit integer or double-double floating-point—see Section 6.2.1)?

(g) Implement this scheme on a parallel computer, preserving the property that the overall sequence of pseudorandom numbers generated by all processors is identical to that generated by a single-processor program. This property is important in parallel computing not only for debugging purposes, but also to permit flexibility in the number of processors used. \( \text{Hint: Note that each processor can independently calculate the starting value of its assigned segment of the sequence. See also Exercise 17 of Chapter 3.} \)

9. **Chaitin’s (Omega) constant.** Chaitin’s constant is perhaps the most compact information theoretic way to encode undecidability via the halting problem for Turing machines. One common accounting of this is as follows. Fix a prefix-free universal Turing machine \( U \): (i.e., if instances \( U(p) \) and \( U(q) \) each halt, then neither \( p \) nor \( q \) is a prefix of the other.) Then Chaitin’s Omega is defined by

\[
\Omega = \sum_{\{U(p) \text{ halts}\}} 2^{-|p|}.
\]

Despite being intrinsically incomputable, the first 64 binary digits of this version of Chaitin’s constant are

000000100000010000001100011010000011110011101101000010000,

as has been recently established in [65].
10. Transcendentality and irrationality.

(a) Prove that \( \log_a b \) and \( a^{1/b} \) are irrational except in the obvious cases.

(b) Prove that \( e \) is irrational by considering

\[
\left| \frac{p}{q} - \sum_{n=0}^{q} \frac{1}{n!} \right| < \frac{1}{q^2 q!}.
\]

(c) More generally, prove that \( \sum_{n \geq 0} (\pm 1) \frac{n}{n!} \) is irrational for all choices of \((\pm 1)_n\), thus explicitly constructing continuum-many irrational numbers.

(d) Establish Liouville’s theorem that if \( \alpha \) is algebraic of degree \( n \), then for all \( \epsilon > 0 \) and all \( c > 0 \)

\[
0 < \left| \alpha - \frac{p}{q} \right| < \frac{c}{q^{n+\epsilon}}
\]

has only finitely many solutions with \( p \) and \( q \) integer.

(e) Deduce that \( \sum_{n \geq 0} (\pm 1) \frac{n}{10^{n!}} \) is transcendental for all choices of \((\pm 1)_n\), thus explicitly constructing an uncountably infinite class of transcendental numbers.

11. The Copeland-Erdős constant. This is 0.2357113171923…, obtained by concatenating the primes. It is sequence A033308 in Sloane’s online sequence encyclopedia. This and other information may be found by entering the decimal in the Inverse Symbolic Calculator. In 1946, Copeland and Erdős showed that it is 10-normal.

12. Paul Erdős, a life that added up to something. In 1996 the mathematical community lost a brilliant and beloved colleague. Here are excerpts from an essay written by Charles Krauthammer of the Washington Post [133]:

One of the most extraordinary minds of our time has left. “Left” is the word Paul Erdős, a prodigiously gifted and productive mathematician, used for “died.” “Died” is the word he used to signify “stopped doing math.” Erdős never died. He continued doing math, notoriously a young person’s field, right until the day he died Friday, Sept. 20. He was 83. . .

He had no home, no family, no possessions, no address. He went from math conference to math conference, from university to university, knocking on the doors of mathematicians throughout
the world, declaring “My brain is open” and moving in. His
colleagues, grateful for a few days collaboration with Erdős—
his mathematical breadth was as impressive as his depth—took
him in.

Erdős traveled with two suitcases, each half-full. One had a
couple of clothes; the other, mathematical papers. He owned nothing
else. Nothing. His friends took care of the affairs of everyday
life for him—checkbook, tax returns, food. He did numbers. . . .

His Washington Post obituary ends with this abrupt and rather
painful line: “He leaves no immediate survivors.”

But in reality he did: hundreds of scientific collaborators and
1,500 mathematical papers produced with them. An astonish-
ing legacy in a field where a lifetime product of 50 papers is
considered extraordinary.

Mathematicians tend to bloom early and die early. The great In-
dian genius, Srinivasa Ramanujan, died at 32. The great French
mathematician, Evariste Galois died at 21. (In a duel. The
night before, it is said, he stayed up all night writing down
everything he knew. Premonition?) And those who don’t liter-
ally die young, die young in Erdős’ sense. By 30, they’ve lost
it.

Erdős didn’t. He began his work early. At 20 he discovered
a proof for a classic theorem of number theory (that between
any number and its double must lie a prime, i.e., indivisible,
number). He remained fecund till his death. Indeed, his friend
and benefactor, Dr. (of math, of course) Ron Graham, estimates
that perhaps 50 new Erdős papers are still to appear.

Erdős was unusual in yet one other respect. The notion of the
itinerant, eccentric genius, totally absorbed in his own world of
thought, is a cliche that almost always attaches to the adjective
“anti-social.” From Bobby Fischer to Howard Hughes, obsession
and misanthropy seem to go together.

Not so Erdős. He was gentle, open and generous with others.
He believed in making mathematics a social activity. Indeed, he
was the most prolifically collaborative mathematician in history.
Hundreds of colleagues who have published with him or been
advised by him can trace some breakthrough or insight to an
evening with Erdős, brain open.
The picture of Paul Erdős in Figure 4.2 captures him very well. It is shown at Grossman’s Erdős Number Project (see http://www.oakland.edu/enp/) Using this online tool, one finds, for example, that there are three Borweins with “Erdős number two,” which connotes that they each wrote a paper with some direct co-author of Erdős, but not with Erdős himself. One also finds that Roland Girgensohn has Erdős number two, and that David Bailey has Erdős number three.
4. Normality of Numbers
The Power of Constructive Proofs I

A proof is a proof. What kind of a proof? It’s a proof. A proof is a proof. And when you have a good proof, it’s because it’s proven.


The advent of the modern computer mathematics systems makes much previously elusive material tangible and certainly helps drive a taste for the concrete. Even when not explicitly using such software, a constructive computational approach to mathematical proofs and derivations is often significantly more enlightening and intuition-promoting than purely abstract approaches. Illustrating both the power and the pleasure of these constructive approaches is the aim of this chapter.

5.1 The Fundamental Theorem of Algebra

We will start this chapter with a proof of the Fundamental Theorem of Algebra, as an experimental mathematician might construct. Let \( p \) be a polynomial defined on the complex plane \( \mathbb{C} \):

\[
p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n. \quad (5.1)
\]

Suppose that \( p(x) \) has no roots in \( \mathbb{C} \). For some sufficiently large \( s \), we can assume \( |p(x)| > 1 \) for all \( x \) with \( |x| \geq s \), because for sufficiently large \( x \), the \( x^n \) term dominates. Since \( |p(x)| \) is continuous on the interior and boundary of the circle with radius \( s \), it follows from fundamental continuity axioms that \( |p(x)| \) achieves a minimum value at a point \( t \) in this (solid) circle. We will see numerous examples in subsequent sections of this “min/max” or “variational” approach in action. Now write

\[
q(z) = p(z - t) = q_0 + q_1 z + \cdots + q_n z^n. \quad (5.2)
\]

Presumably the polynomial \( q \) has a global minimum \( M \) at \( 0 \), and \( M = |q_0| = |q(0)| > 0 \).
Our proof strategy is to construct some point $x$, close to the origin, such that $|q(x)| < |q(0)|$, thus contradicting the presumption that $q$ has a global minimum at zero. One idea that immediately suggests itself to the experimental mathematician is to employ Newton’s method, for finding roots of a function $f$. This is the well-known scheme in which we choose $x_0$ to be some initial value, and then iterate

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

(see Section 6.2.5). One detail that needs to be observed here is how to handle the case where the derivative in Newton’s iteration (5.3) is zero. In that case we simply adapt a higher-order approximation from the Taylor’s series of the function $f(x)$. In particular, if the first $m$ derivatives of $f(x)$ at $x_k$ are zero, but not the $(m+1)$-st derivative, then we can write

$$x_{k+1} = x_k + \left( \frac{-m! f(x_k)}{f^{(m)}(x_k)} \right)^{1/m},$$

where the $m$-th root of a complex number $z = ae^{ib}$ is calculated using the well-known formula

$$z^{1/m} = a^{1/m} (\cos(b/m) + i \sin(b/m)).$$

In general we have no global guarantee that $x_{k+1}$ is closer to the root than $x_k$, but for the purposes of our present proof strategy, we do not require this—we only require some point $x$ whose function value is slightly smaller than the function value at zero. If Newton’s method gives us merely a direction in the complex plane for which the function value decreases in magnitude (a descent direction), then by moving a small distance in that direction, we hope to achieve our goal of exhibiting a complex $x$ such that $|q(x)| < |q(0)|$. This is the strategy we will pursue.

So suppose that the first nonzero coefficient of $q$, following $q_0$, is $q_m$ (if there is no nonzero coefficient following $q_0$, then the polynomial reduces to a constant):

$$q(x) = q_0 + q_m x^m + q_{m+1} x^{m+1} + \cdots + q_n x^n.$$  

(5.6)

Note that $q^{(m)}(x) = m! q_m$. Thus, in accordance with (5.4), we will choose $x$ to be the complex number

$$x = r \left( \frac{-q_0}{q_m} \right)^{1/m}.$$  

(5.7)
5.1. The Fundamental Theorem of Algebra

for some small positive real \( r \) that we will specify below. Now we can write

\[
q(x) = q_0 - q_0 r^m + q_{m+1} r^{m+1} \left( -\frac{q_0}{q_m} \right)^{1+1/m} + \cdots + q_n r^n \left( -\frac{q_0}{q_m} \right)^{n/m} = q_0(1 - r^m) + \mathcal{E},
\]

where the error term \( \mathcal{E} \) satisfies

\[
|\mathcal{E}| \leq \frac{r^{m+1} \max |q_i|}{1 - s} \left| \frac{q_0}{q_m} \right|^{1+1/m}
\]

for \( s = r |q_0/q_m| \), which is smaller than one when \( r \) is sufficiently small. In this way, \( \mathcal{E} \) can be made arbitrarily small in ratio to \( |q_0|r^m \) by choosing \( r \) small enough. Thus, for such an \( r \), we have \( |q(x)| = |q(0)(1 - r^m) + \mathcal{E}| < |q(0)| \), which contradicts our original assumption that \( q(x) \) has a global minimum at zero.

This establishes the Fundamental Theorem of Algebra. Continuing by induction, we have constructively proven:

**Theorem 5.33.** Every complex polynomial of degree \( n \) has exactly \( n \) complex roots.

More importantly, we have gained some modest insight into how to practically locate roots. Indeed, a careful scheme along these lines can lead to a fairly robust numerical procedure for finding polynomial roots (this is discussed more in Section 7.3 of the second volume of this work).

5.1.1 Liouville’s Theorem and the Sine Product

Of course, depending on what tools we consider elementary, other proofs may seem equally or more transparent. Suppose we are familiar with the following generalization of the Fundamental Theorem of Algebra, an application of the Cauchy-Goursat theorem:

**Theorem 5.34.** (Liouville). Every entire function in the complex plane with polynomial growth of degree at most \( n \) is a polynomial of degree at most \( n \).

Then the assumption that

\[
p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n
\]

never vanishes leads almost immediately to the Fundamental Theorem of Algebra.
We illustrate the use of Theorem 5.0 by deriving the product formula for the \( \sin \) function (5.41). This will be discussed more completely in Section 5.4. We begin by considering

\[
\sigma(z) = \pi z \prod_{n=1}^{\infty} \left( 1 - \frac{z^2}{n^2} \right), \tag{5.10}
\]

for \( z \in \mathbb{C} \), and analyzing the quotient

\[
q(z) = \frac{\sigma(z)}{\sin(\pi z)}. \tag{5.11}
\]

We rewrite \( \sigma \) as

\[
\sigma(z) = \pi z(1 - z) \prod_{n=1}^{\infty} \left( 1 + \frac{z(1 - z)}{n(n+1)} \right),
\]

by gathering the terms in \( 1 + z/n \) and \( 1 - z/(n+1) \) together. This shows that \( \sigma(1 - z) = \sigma(z) \) and so that \( \sigma(z + 1) = -\sigma(z) \). Thus, \( q \) is entire as both numerator and denominator have simple zeroes at the integers and are pole free. Moreover,

\[
q(z + 1) = q(z),
\]

and

\[
q(n) = q(0) = \lim_{z \to 0} \frac{\sin(z)}{z} = 1, \tag{5.12}
\]

for each integer \( n \). It remains to bound \( q \). First, we write

\[
\left| \prod_{n=1}^{\infty} \left( 1 - \frac{z^2}{n^2} \right) \right| \leq \exp \left( \sum_{k=1}^{\infty} \log \left( 1 + \frac{|z|^2}{k^2} \right) \right) \tag{5.13}
\]

\[
\leq \exp \left( \log(1 + |z|^2) + \int_1^{\infty} \log \left( 1 + \frac{|z|^2}{u^2} \right) du \right)
\]

\[
= \exp(\pi |z| - 2|z| \arctan(1/|z|)) \leq \exp(\pi |z|).
\]

Then we observe that, as \( q \) has period 1, it suffices to establish that

\[
|q(z)| \leq a |z| + b, \text{ when } -1/2 \leq \text{Re}(z) \leq 1/2 \tag{5.14}
\]

for some \( a, b > 0 \). Once (5.14) is established, Theorem 5.0 ensures that \( q \) is at most linear, but as \( q \) takes the value 1 infinitely often, \( q(z) \equiv 1 \) and
5.1. The Fundamental Theorem of Algebra

we are done. To establish Equation (5.14), let us write $x$ and $y$ for the real and imaginary parts of $z$. We note that

$$\inf_{|x|, |y| \leq 1/2} \left| \frac{\sin z}{z} \right| > 0 \quad (5.15)$$

as $\sin$ has zeroes only at the integers, while for $|x| \leq 1/2$ and $|y| \geq 1/2$ we have

$$|\sin(\pi z)| \geq |\sinh(\pi |y|)| \geq c \exp(\pi |z|) - d, \quad (5.16)$$

for $c, d > 0$. Combining these last two estimates with that of (5.10) produces (5.14).

Even if we distrust and only partially understand Theorem 5.0, and we perform the steps in the previous proof informally, we finish with greater security that the result is true and more reason to search for a compelling and constructive proof.

That said, computer algebra systems are not perfect and this seems an appropriate place to highlight one of the issues most vexing for symbolic computation—selecting the right branch of the inverse of a function.

5.1.2 Roots and Branches

We start with two “failures”:

**Example 5.35.** Simplifying $\sqrt{x}$.

Evaluating asymptotic expansions for the Airy function (the first solution of $w'' - zw = 0$, which one can see in the rainbow), Rob Corless and Dave Jeffrey could not get correct values for negative $x$, in *Maple* version 4 (circa 1988).

The problem turned out to be in the calculation of $\sqrt{-x}$.

*Maple* was “simplifying” automatically

$$\sqrt{-x} \rightarrow i \sqrt{x},$$

and therefore when it tried substituting, say, $x = -4$ it computed as follows.

$$\sqrt{-x} \rightarrow i \sqrt{-4}; \quad i \sqrt{-4} \rightarrow i \sqrt{4} = 2; \quad i \sqrt{4} = 2 \rightarrow 2.$$

Of course, they wanted $\sqrt{-(-4)} = 2$. Corless and Jeffrey’s quick fix was to program
temp:= -x; sqrt(temp);

The slow fix was to identify a set of problems called generically by Maple developers as “The Square Root Bug.” Of course, humans routinely write $\sqrt{x^2} = x$ and worry about it afterwards.

Example 5.36. Simplifying $\sin(\arcsin(x))$.

One computer algebra system simplified $\sin(\text{asin}(5/4)) \rightarrow -5/4$ using the “standard” formulae:

$$\arcsin z = \arctan \left( \frac{z}{\sqrt{1 - z^2}} \right)$$

(5.17)

$$\sin (\arctan z) = \frac{z}{\sqrt{z^2 + 1}}.$$  

(5.18)

and internally used (5.17) to convert inverse sine to inverse tangent:

$$\arcsin(5/4) = \arctan(-5i/3).$$

The system then used (5.18), with the complex number, and got the wrong sign:

$$\frac{-5i/3}{\sqrt{5^2(-1)/3^2 + 1}} = \frac{-5i/3}{\sqrt{-16/9}} = -5/4.$$

This time the cure was to modify

$$\arcsin z = \arctan \left( \frac{z}{\sqrt{1 - z^2}} \right)$$

(5.19)

$$\sin (\arctan z) = \frac{z}{\sqrt{z^2 + 1}} = \frac{1}{\sqrt{z^2 + 1}}$$

(5.20)

to

and to ensure that

$$\sqrt{\frac{1}{z}}$$

was not automatically simplified to $\frac{1}{\sqrt{z}}$. 

\qed
5.1. The Fundamental Theorem of Algebra

Additionally, the different systems and reference books do not necessarily agree on what the domain of arcsin is (even, for example, in different editions of Abromowitz and Stegun [1]), or where the branch cut for log occurs.

These and other examples show how errors may be caused by any of the following

\[
\sqrt{xy} \to \sqrt{x} \sqrt{y}, \quad \sqrt{x^2} \to x, \\
\sqrt{\frac{1}{z}} \to \frac{1}{\sqrt{z}}, \quad \log(e^z) \to z, \\
\log(1/z) \to -\log z, \quad \arctan z = \arcsin \left(\frac{z}{\sqrt{z^2 + 1}}\right),
\]

being used in simplifications.

The source of the problems is that in the complex plane, functions such as log, square root, are multi-valued. In each problematic transformation, at least one multi-valued function is being manipulated in the complex plane using a law that applies to the single-valued function defined for real, positive arguments. The issue becomes how to treat multivalued functions (i) in human mathematics, and (ii) in a computer system.

Many solutions have been proposed:

Example 5.37. Simplifying $\log AB$.

Consider the relation

\[
\log(AB) = \log A + \log B .
\]

Maple proves this is wrong by substituting $A = B = -1$.

\[
> eq := \log(A*B) = \log(A) + \log(B) ; \\
> eq := \ln(A \ B) = \ln(A) + \ln(B) \\
> subs(A=-1,B=-1),eq ; \\
> \ln(1) = 2 \ \ln(-1) \\
> simplify(%) ; \\
0 = 2 \ \mathrm{I} \ \Pi
\]

Many people are quite unhappy with this. They reply either (i) Abramowitz and Stegun define the multivalued function Log (a Principal Value) and this is the function to use: the correct equation should be

\[
\log(AB) = \log A + \log B ;
\]
or (ii) they observe that the trouble is that Maple is not working on the Riemann surface, and if it did, all its problems would be solved.

To explain these responses, several terms need to be specified. A \textit{multi-valued function} is a function (e.g., log, inverse sine, square root) that can, in principle, have multiple values associated with it. A function returning \textit{multiple values} is a multivalued function that is defined to return more than one value. The values might be returned as a set or in some other data structure. A \textit{principal-valued} function is a selection of multivalued function that specifies a single preferred value. Corless and Jeffrey then asked whether \(\log(-1)\) represents the single number \(i\pi\)? All the solutions \(z\) of the equation \(\exp(z) = -1\), as the set \(\{i\pi + 2\pi k \mid k \in \mathbb{Z}\}\)? Some object in between these two, perhaps a single number \(i\pi + 2\pi k\) with the value of \(k\) being fixed later?

A traditional response was provided by Carathéodory writing on the equation
\[
\log z_1 z_2 = \log z_1 + \log z_2, \tag{5.21}
\]
for complex \(z_1, z_2\).

The equation merely states that the sum of one of the (infinitely many) logarithms of \(z_1\) and one of the (infinitely many) logarithms of \(z_2\) can be found among the (infinitely many) logarithms of \(z_1 z_2\), and conversely every logarithm of \(z_1 z_2\) can be represented as a sum of this kind (with a suitable choice of \(\log z_1\) and \(\log z_2\)).

The above definition is not an equality between sets. Consider a special case of \(3\log z = \log z^3\).
\[
3\log(-1) = \log((-1)^3) = \log(-1).
\]
The left-hand side is the set \(\{3i\pi + 6i\pi k\}\), but the right-hand is the set \(\{i\pi + 2i\pi k\}\). Also, mathematically, \(\log z\) does not have a unique value, while computer algebra systems accept a specific value for \(z\) and return a unique \(\log z\). From another point of view, the value of \(\log z\) is no longer determined solely by the value of \(z\): The value to be given to \(\log z\) is also determined by the context. Thus, if the left-hand side \(\log(-1)\) equals \(i\pi\), then the right-hand \(\log(-1)\) equals \(3i\pi\).

Multiple values are not computational as working with the solution of the cubic equation \(z^3 + 3qz - 2r = 0\) shows. In keeping with Carathéodory, the solution by radicals, ascribed to Cardano (1501–1576) and Tartaglia (1499–1557), is written as
\[
z = \left( r + (r^2 + q^3)^{1/2} \right)^{1/3} + \left( r - (r^2 + q^3)^{1/2} \right)^{1/3}.
\]
Each square root has two values and each cube root has three, and each
term in the addition takes an independent value. Even allowing for sym-
metry, \( z \) is elected from a set of more than three possible \( z \).

Jeffrey writes:

Traditionally, this inefficiency has not bothered human mathemati-
cians, who patiently try all the solutions until the three correct ones
are verified, but it is not desirable in a computer system.

He likewise argues against using Riemann surfaces (others disagree) and
ends up recommending the use of principal values in computer systems,
with labeled branches to express multivaluedness better, and the use of the
so-called unwinding number, [121] [75], to keep transformations correct. In
conclusion he appropriately notes that there is reluctance to give up the
old formulae

\[
\left( \left( \left( \left( z^2 \right)^{1/2} \right)^3 \right)^{1/3} \right)^4 = z
\]

and that there are limits to what computer algebra systems can introduce,
unilaterally, in the way of new mathematical ideas and notation. We refer
the reader to [74] for a fuller discussion of the issues in “reasoning about
the elementary functions of complex analysis.”

When a program returns a patently negative value for an area or a
complex number in a real integral, any alert user will be flagged. While
numerical checking will help, it is much more invidious when simplification
of an expression takes a wrong branch internally, but returns, say, \( \log(7/9) \)
when the right answer is \( \log(4/5) \).

Suffice it to say that the user of any system should be alert to such issues
and on the inherent difficulties in addressing the underlying problems.

5.2 The Uncertainty Principle

In this section, we illustrate in detail how one may be led to a larger
discovery by directed computation and visualization.

Some readers may be familiar with the uncertainty principle from quan-
tum mechanics, which is often expressed as the fact that the position and
momentum of a subatomic-scale particle cannot simultaneously be pre-
scribed or measured to arbitrary accuracy. Other readers may be familiar
with the uncertainty principle from signal processing theory, which is often
expressed as the fact that a signal cannot simultaneously be “time-limited”
and “frequency-limited.” Remarkably, the precise mathematical formulations of these two principles are identical.

Richard Crandall illustrates the uncertainty principle with a “thought experiment.” Imagine that a tuning fork is struck, then very quickly silenced—just a brief burst of sound. If the duration \( \Delta t \) is short enough, the perceived pitch would be ambiguous, so that the “uncertainty” in the frequency \( \Delta f \) would be large. More precisely, the spectrum of such a sound, if viewed on a spectrum analyzer, would be rather broad. If the duration is long, then the listener (and the spectrum analyzer) can hear enough cycles of the signal to gauge the pitch quite accurately, in which case \( \Delta f \) is small—the spectrum would be sharply peaked at the tuning fork’s natural frequency. Thus we can write \( \Delta t \Delta f > C \) for some constant \( C \). This is the basic idea of the uncertainty principle.

The most common proof of the uncertainty principle is not terribly difficult, although it is hardly intuitive (and certainly not very enlightening) at first reading. We will sketch it here, assuming some elementary facts of analysis. Let us consider a real, continuously differentiable, \( L^2 \) function \( f(t) \), which further satisfies \( f(t) \sqrt{t} \to 0 \) as \( |t| \to \infty \). For convenience, we will also assume here that \( f(-t) = f(t) \), as this insures that the Fourier transform \( \hat{f}(x) \) of \( f(t) \) is purely real, although in general this condition is not necessary. Define (see also Section 2.2 of the second volume):

\[
\begin{align*}
E(f) &= \int_{-\infty}^{\infty} f^2(t) \, dt \\
V(f) &= \int_{-\infty}^{\infty} t^2 f^2(t) \, dt \\
\hat{f}(x) &= \int_{-\infty}^{\infty} f(t) e^{-itx} \, dt \\
Q(f) &= \frac{V(f)}{E(f)} \cdot \frac{V(\hat{f})}{E(\hat{f})}.
\end{align*}
\] (5.22)

**Theorem 5.38.** With the above assumptions and definitions, \( Q(f) \geq 1/4 \), with equality if and only if \( f(t) = ae^{-(bt)^2/2} \) for real constants \( a \) and \( b \).

**Proof.** By applying the integral form of the Schwarz inequality [1 pg. 256] (see also formula (5.32)), to the functions \( tf(t) \) and \( f'(t) \), we can write

\[
\left| \int_{-\infty}^{\infty} tf(t)f'(t) \, dt \right|^2 \leq \left[ \int_{-\infty}^{\infty} t^2 f^2(t) \, dt \right] \left[ \int_{-\infty}^{\infty} (f'(t))^2 \, dt \right]. \tag{5.23}
\]
5.2. The Uncertainty Principle

Furthermore,

\[ \int_{-\infty}^{\infty} tf(t)f'(t) \, dt = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d}{dt} f^2(t) \, dt = -\frac{1}{2} E(f) \quad (5.24) \]

by applying integration by parts. Let \( g(t) = f'(t) \). By noting that \( \hat{g}(x) = -ix\hat{f}(x) \), and by applying Parseval’s identity \[162\] pg. 65 to \( f(t) \) and \( g(t) \), we obtain, respectively,

\[
\int_{-\infty}^{\infty} |f(t)|^2 \, dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} |\hat{f}(x)|^2 \, dx \\
\int_{-\infty}^{\infty} |f'(t)|^2 \, dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} x^2 |\hat{f}(x)|^2 \, dx. \quad (5.25)
\]

Combining these results, we obtain our desired inequality. Recall that equality in the Schwarz inequality occurs only when the two functions (\( tf(t) \) and \( f'(t) \) in this case) are linear scalings of each other, i.e., \( f'(t) = ctf(t) \) for some \( c \). By solving this elementary differential equation, we conclude that the minimum value \( 1/4 \) is achieved if and only if \( f(t) = ae^{-(bt)^2/2} \) for constants \( a \) and \( b \), or in other words for a scaled Gaussian probability density function. By the way, it is worth noting that \( Q(f) \) is unaffected by a linear scaling of either the function argument \( t \) or the function value \( f(t) \).

Now let us approach this problem as an experimental mathematician might. As was mentioned above, it is natural when studying Fourier transforms (particularly in the context of signal processing) to consider the “dispersion” of a function and to compare this with the dispersion of its Fourier transform. Noting what appears to be an inverse relationship between these two quantities, we are naturally led to consider the expression

\[ Q(f) = \frac{V(f)}{E(f)} \cdot \frac{V(\hat{f})}{E(\hat{f})}. \quad (5.26) \]

With the assistance of Maple or Mathematica, we can readily work out some examples, as shown in Table 5.1. We note that each of the entries in the last column of the table is in the range \((1/4, 1/2)\). For example, the expression in the bottom right corner of the table is approximately 0.26329. Can we get any lower?

To further study this problem with an experimental approach, we employ numerical methods, since these permit the above calculations to be performed for a wide variety of functions, analytic or tabular. We can...
do this by approximating the Fourier transform \( \hat{f}(x) \) by means of a step-function approximation to the integral, as follows (see also Section 6.1). Assume that \( f(t) \) is zero (or sufficiently small) outside \([-a/2, a/2]\), and its Fourier transform \( \hat{f}(x) \) is zero (or sufficiently small) outside \([-b/2, b/2]\). Select an even integer \( n \) so that \( ab = 2\pi n \). This usually requires that we adjust \( a \) and \( b \) to be larger than the minimum values needed, particularly if a large value of \( n \) is needed for high accuracy in the approximation. \( n \) is typically chosen to be a power of two. Then we can write

\[
\hat{f} \left( \frac{bk}{n} \right) = \int_{-\infty}^{\infty} f(t) e^{-i\frac{bk}{n}t} dt \\
\approx \frac{a}{n} \sum_{j=1}^{n-1} f \left( \frac{aj}{n} \right) e^{-i\frac{aj}{n}(bk/n)}
\]

for \(-n/2 + 1 \leq k \leq n/2\). If we adopt the convention that \( f(t) = f(t-a) \) for \( t > a/2 \), and \( \hat{f}(x) = \hat{f}(x-b) \) for \( x > b/2 \), then we can write

\[
\hat{f} \left( \frac{bk}{n} \right) = \frac{a}{n} \sum_{j=0}^{n-1} f \left( \frac{aj}{n} \right) e^{-2\pi ijk/n},
\]

for \( 0 \leq k \leq n-1 \), which is now in a form suitable for the application of widely available fast Fourier transform (FFT) routines.

The integrals in the definition of \( Q \) can now be computed using similar step-function approximations, as follows:

<table>
<thead>
<tr>
<th>( f(t) )</th>
<th>Interval</th>
<th>( \hat{f}(x) )</th>
<th>( E(f) )</th>
<th>( V(f) )</th>
<th>( V(\hat{f}) )</th>
<th>( Q(f) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 1 - t ) sgn(t)</td>
<td>([-1, 1])</td>
<td>(2(1 - \cos x)/x^2)</td>
<td>2/3</td>
<td>1/15</td>
<td>4\pi</td>
<td>3/10</td>
</tr>
<tr>
<td>( 1 - t^2 )</td>
<td>([-1, 1])</td>
<td>(4(\sin x - x \cos x)/x^3)</td>
<td>16/15</td>
<td>16/105</td>
<td>16\pi/3</td>
<td>5/14</td>
</tr>
<tr>
<td>( 1/(1 + t^2) )</td>
<td>([-\infty, \infty])</td>
<td>(\pi \exp(-x \text{ sgn} x))</td>
<td>(\pi/2)</td>
<td>(\pi/2)</td>
<td>(\pi^2/2)</td>
<td>1/2</td>
</tr>
<tr>
<td>( e^{-</td>
<td>t</td>
<td>} )</td>
<td>([-\infty, \infty])</td>
<td>(2/(1 + x^2))</td>
<td>1</td>
<td>1/2</td>
</tr>
<tr>
<td>( 1 + \cos t )</td>
<td>([-\pi, \pi])</td>
<td>(2\sin(\pi x)/(x - x^3))</td>
<td>(3\pi)</td>
<td>(\pi^3 - 15\pi/2)</td>
<td>2\pi^2</td>
<td>(\pi^2 - 15/2)/9)</td>
</tr>
</tbody>
</table>

Table 5.1. \( Q \) values for various functions.
5.2. The Uncertainty Principle

\[
E(f) = \int_{-\infty}^{\infty} f^2(t) \, dt \approx \frac{a}{n} \sum_{j=-n+1}^{n} f^2 \left( \frac{aj}{n} \right)
\]

\[
V(f) = \int_{-\infty}^{\infty} t^2 f^2(t) \, dt \approx \frac{a}{n} \sum_{j=-n+1}^{n} \left( \frac{aj}{n} \right)^2 f^2 \left( \frac{aj}{n} \right)
\]

\[
E(\hat{f}) = \int_{-\infty}^{\infty} \hat{f}^2(x) \, dx \approx \frac{b}{n} \sum_{j=-n+1}^{n} \hat{f}^2 \left( \frac{bj}{n} \right)
\]

\[
V(\hat{f}) = \int_{-\infty}^{\infty} x^2 \hat{f}^2(x) \, dx \approx \frac{b}{n} \sum_{j=-n+1}^{n} \left( \frac{bj}{n} \right)^2 \hat{f}^2 \left( \frac{bj}{n} \right), \quad (5.30)
\]

where we use the results of the FFT scheme for the indicated array of \( \hat{f} \) values.

Given an equispaced array \( (t_k) \) with spacing \( d \), and a corresponding array \( (y_k) \), define \( f(t) \) to be the function given by parabolic interpolation in the \( (y_k) \) array. To be precise, this means that for \( t \) in the interval \( (t_k, t_{k+1}) \), define \( f(t) = y_k - h(3y_k - 4y_{k+1} + y_{k+2})/2 + h^2(y_k - 2y_{k+1} + y_{k+2})/2 \), where \( h = (t-t_k)/d \). We can now employ a simple search strategy to explore the space of continuous functions to find one that minimizes \( Q \):

**Algorithm 5.39.** To find a \( Q \)-minimizing function \( f(t) \):

Given \( c \) and \( m \), first construct the \( (m+3) \)-long abscissa array \( (t_k = ck/m) \), for \( 0 \leq k \leq m + 2 \), which has spacing \( d = c/m \). Define the tent-function array \( (y_k = 1 - k/m) \) for \( 0 \leq k \leq m \), with \( y_{m+1} = y_{m+2} = 0 \). Define \( f(t) \) as above based on the \( (y_k) \) array. For negative \( t \), define \( f(t) = f(-t) \), and define \( f(t) = 0 \) for \( |t| > c \). Initially set \( \delta \) to be some small value, and calculate \( Q_{\text{min}} = Q(f) \), utilizing the scheme described above, for \( f(t) \) as just defined. Now iterate as follows: Starting with \( k = 1 \) (not \( k = 0 \)), increase \( y_k \) by \( \delta \) (leaving other \( y_j \) unchanged) and calculate \( Q(f) \) for \( f(t) \) associated with this altered \( y \) array. If \( Q(f) < Q_{\text{min}} \), then replace \( Q_{\text{min}} \) by \( Q(f) \), and replace the \( y \) array with the altered \( y \) array; if not, then decrease \( y_k \) by \( \delta \), and replace as before if \( Q(f) < Q_{\text{min}} \). Either way, increment \( k \) and perform similar tests until the case \( k = m \) is complete. If for some \( k \) the test \( Q(f) < Q_{\text{min}} \) was true, then repeat beginning with \( k = 1 \). If not, then reduce \( \delta \) by a factor of two and start again. Terminate when \( \delta \) is sufficiently small. \( \Box \)
In our implementation of this procedure, we use the parameters $a = 128$, $b = 64\pi$, and $n = 4096$ for the FFT and integration procedures (so that $ab = 2\pi n$ as required in the FFT). In the search procedure, we set $c = 8$ and $m = 32$. We set the initial $\delta = 1/16$, and we terminate when $\delta < 10^{-6}$. This requires about 30 minutes on a 2003-era personal computer or workstation. An acceptable, but less accurate, result is obtained in just a minute or so by using the termination condition $\delta < 10^{-4}$.

The final experimentally determined $Q$-minimizing function $f(t)$ that we obtain is plotted in Figure 5.1. Needless to say, its shape strongly suggests a Gaussian probability curve. Actually, we have graphed both $f(t)$ and the function $e^{-\frac{(bt)^2}{2}}$, where $b = 0.45446177$, on the same plot—they are identical to the precision of the plot! We graphed the difference between these two functions in Figure 5.2. The value of $Q$ corresponding to this $f(t)$ is $0.25001158$, which indeed is very close to $1/4$.

If you do calculations of this sort, you may discover a curious fact. When the numeric computational scheme described above (which is based on discrete, step-function approximations for the various integrals involved) is applied to compute $Q$ for a scaled Gaussian function (namely a function of the form $ae^{-\frac{(bt)^2}{2}}$), the result of this calculation is very accurate. The value of $Q$ produced by our program is $1/4$, correct to 15 decimal places (using ordinary IEEE double floating-point arithmetic), even with a modest value of $n$. For other types of functions, with a step-function interval of $10^{-4}$ or so, typically only six or seven digits are good.

What is happening here is that we have experimentally uncovered an important and nontrivial fact of numerical analysis: If a function $f(t)$ and all its derivatives approach zero as $t$ approaches the endpoints of the interval $[a, b]$ (which condition is certainly satisfied by the Gaussian probability density function on $(-\infty, \infty)$), then calculating the definite integral of $f(t)$ on $[a, b]$ by means of a simple step-function or trapezoidal approximation scheme is extraordinarily accurate [9, pg. 280]. This fact, which is a consequence of the Euler-Maclaurin summation formula, is the basis of some new robust and high-precision numerical quadrature algorithms. We shall discuss these schemes, plus the Euler-Maclaurin summation formula, in Section 7.4 of the second volume.

5.3 A Concrete Approach to Inequalities

Discovering and establishing inequalities underpins much of mathematics. It has been claimed that most of analytic number theory is the Cauchy-Schwarz inequality in various disguises. Its ubiquitous extension is Hölder’s
Figure 5.1. Experimental $Q$-minimizing function and matching Gaussian.

Figure 5.2. Difference between $Q$-minimizing function and matching Gaussian.
inequality. For $1 \leq p, q \leq \infty$, we define the $p$–norm of a sequence in $\mathbb{R}^n$

$$\|x\|_p = \sqrt[p]{\sum_{k=1}^{n} |x_k|^p}.$$ 

For $p = \infty$, the norm is $\|x\|_\infty = \max_{k=1}^{n} |x_k|$, which coincides with $\lim_{p \to \infty} \|x\|_p$. We use $\langle x, y \rangle$ for the dot-product.

**Theorem 5.40.** If $1/p + 1/q = 1$ then

$$\langle x, y \rangle \leq \|x\|_p \|y\|_q,$$  

(5.31)

with equality only if $x_k$ and $y_k$ are “aligned” (i.e., $x = cy$ for some scalar $c$).

**Proof.** We may assume $x$ and $y$ are nonzero. We proceed in several steps. First, we establish the Fenchel-Young inequality

$$\frac{1}{p} |x|^p + \frac{1}{q} |y|^q \geq xy$$

for real $x$ and $y$. This can be done by observing that it suffices to assume $x, y$ are positive and to use calculus on the function $x \mapsto (x^p)/p + (y^q)/q - xy$, which has a critical point at 0 and is convex. Then we have

$$\sum_{k} \left( \frac{1}{p} x_k^p + \frac{1}{q} y_k^q \right) \geq \sum_{k} x_k y_k,$$

which is

$$\frac{1}{p} \|x\|_p^p + \frac{1}{q} \|y\|_q^q \geq \langle x, y \rangle.$$

In particular if $z = x/\|x\|_p^p$, and $w = y/\|y\|_q^q$, we deduce that $\langle z, w \rangle \leq 1$ as each of $w, z$ are unit length and $1/p + 1/q = 1$. This establishes (5.31).

We leave the proof of the equality statement to the reader. They emerge on analyzing when the Fenchel-Young inequality is an equality. □

The corresponding integral inequality

$$\int_R x(t)y(t) dt \leq \left[ \int_R |x(t)|^p dt \right]^{1/p} \left[ \int_R |y(t)|^q dt \right]^{1/q}$$  

(5.32)

is proven in the same way.
When \( p = q = 2 \), we recover the Cauchy-Schwarz inequality. In general for a function \( f : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\} \), we may define the (Fenchel-Legendre) conjugate by

\[
 f^*(y) = \sup_x \langle x, y \rangle - f(x).
\]

The conjugate is always convex and lower semicontinuous. First used, less explicitly, by Legendre in the study of adjoint systems of ODE’s, \( f^* \) plays a role like the Fourier conjugate in that for convex (lower-semi) continuous functions \( f = f^{**} \), [53]. For example, \( f = x \to x \log(x) - x \) has \( f^* = \exp \) and \( f^{**} = f \). Hence, symbolically performing the code below actually proves that \( f \) is convex. Moreover, the definitional inequality \( f(x) + f^*(y) \geq \langle x, y \rangle \) is what we used in the proof. As we observed in Section 5.1.2, computer algebra systems struggle with branches (i.e., multiple inverses).

Thus, the following Maple code

```maple
conj:=proc(f,y) local x,g:g:=y*x-f(x);
simplify(subs(x=solve(diff(g,x),x)[1],g),symbolic);end;
```

has to be massaged to deal with \( x^p/p \), but is fine with \( x^4/4 \). We have illustrated that convexity is in some sense easy to handle computationally. A much more sophisticated version of the above is detailed next.

**Example 5.41.** A symmetric pair of functions [53].

(a) Given real \( \gamma_1, \gamma_2, \ldots, \gamma_n > 0 \), define \( h : \mathbb{R}^n \to (-\infty, +\infty] \) by

\[
 h(x) = \begin{cases} 
 \prod_{i=1}^{n} x_i^{-\gamma_i} & \text{if } x \in \mathbb{R}^n_+ \\
 +\infty & \text{otherwise.}
\end{cases}
\]

By writing \( g(x) = \exp(\log g(x)) \) and using a composition formula, one can prove that

\[
 h^*(y) = \begin{cases} 
 -(\gamma + 1) \prod_{i=1}^{n} \left(\frac{-y_i}{\gamma_i}\right)^{\gamma_i/\gamma + 1} & \text{if } -y \in \mathbb{R}^n_+ \\
 +\infty & \text{otherwise,}
\end{cases}
\]

where \( \gamma = \sum_i \gamma_i \).

(b) Given real \( \alpha_1, \alpha_2, \ldots, \alpha_n > 0 \), define \( \alpha = \sum_i \alpha_i \) and suppose a real \( \mu \) satisfies \( \mu > \alpha + 1 \). Now define a function \( f : \mathbb{R}^n \times \mathbb{R} \to (-\infty, +\infty] \) by

\[
 f(x, s) = \begin{cases} 
 \mu^{-1} s^\mu \prod_{i} x_i^{-\alpha_i} & \text{if } x \in \mathbb{R}^n_+, \ s \in \mathbb{R}_+ \\
 +\infty & \text{otherwise.}
\end{cases}
\]
Using part (a) one may then prove that
\[
f^*(y, t) = \begin{cases} 
\rho \nu^{-1} \nu \prod_i (-y_i)^{-\beta_i} & \text{if } -y \in \mathbb{R}^n_+, t \in \mathbb{R}_+ \\
+\infty & \text{otherwise}
\end{cases}
\]
for constants
\[
\nu = \frac{\mu}{\mu - (\alpha + 1)}, \quad \beta_i = \frac{\alpha_i - (\alpha + 1)}{\mu}, \quad \rho = \prod_i \left(\frac{\alpha_i}{\mu}\right)^{\beta_i}.
\]
The punch line is that on deducing \( f = f^{**} \), we explicitly represent \( f \) as a convex function. Indeed, one can now show that \( f \) is strictly convex, since \( f^* \) is differentiable.

\[\square\]

5.4 The Gamma Function

The Gamma function naturally extends the factorial and appears throughout this chapter. We begin with a characterization that again exploits convexity. The Gamma function is usually defined as an integral
\[
\Gamma(x) = \int_0^\infty \exp(-t)t^{x-1}\,dt \quad (5.33)
\]
for \( \text{Re}(x) > 0 \).

**Theorem 5.42. (Bohr-Mollerup).** The Gamma function is the unique function \( f : (0, \infty) \rightarrow (0, \infty) \) with the following three properties:

1. \( f(1) = 1 \);
2. \( f(x + 1) = xf(x) \);
3. \( f \) is log-convex (i.e., \( x \rightarrow \log(f(x)) \) is convex).

**Proof.** We sketch the proof. First we show the integral in (5.33) does indeed have the requisite three properties. The first two are easy integration exercises (which can be automated in Maple or Mathematica). For the key property 3, we use the integral version of Hölder’s inequality (5.32) to show that
\[
\sqrt{\Gamma(x)\Gamma(y)} \leq \Gamma\left(\frac{x+y}{2}\right).
\]
5.4. The Gamma Function

Conversely, we set \( g(x) = \log(f(x)) \), we observe that \( g(n+1) = \log(n!) \), and use the convexity estimate

\[
x \log(n) \leq g(n+1 + x) - g(n+1) \leq x \log(n+1)
\]  

for \( 0 < x \leq 1 \).

Hence, for \( 0 < x \leq 1 \),

\[
0 \leq g(x) - \log \frac{n! n^x}{(x+1) \cdots (x+n)} \leq x \log \left( x + \frac{1}{n} \right).
\]

It follows using \( f(x+1) = xf(x) \), that for all \( x > 0 \)

\[
f(x) = \lim_{n \to \infty} \frac{n! n^x}{x(x+1) \cdots (x+n)} = \Gamma(x).
\]  

Equation (5.36) often proves useful in its own right, as we shall see in (5.37) and in (5.44).

Another nice characterization of the Gamma function, which in practice often seems more difficult to apply, is:

**Theorem 5.43.** If \( f \) is a complex valued function on \((a, \infty]\) such that \( f(x+1) = xf(x) \) for all \( x > a \) and

\[
\lim_{n \to \infty} \frac{f(t+n+1)}{n! n^t} = 1
\]

for \( 0 \leq t < 1 \), then \( f = \Gamma \) on \((a, \infty]\).

**Proof.** The fact that \( \Gamma \) satisfies (5.37) is (5.36). Conversely, if \( f \) and \( g \) satisfy (5.37), then consider \( h = f/g \) which satisfies \( \lim_{n \to \infty} h(t+n+1) = 1 \). Since \( h(x) = h(t+n+1) \), the two solutions must both coincide with \( \Gamma \), on \([a, \infty)\).

We illustrate the use of the Bohr-Mollerup Theorem as follows:

**Example 5.44.** The \( \beta \)-function.

The \( \beta \)-function is defined by the integral

\[
\beta(x, y) = \int_0^1 t^{x-1}(1-t)^{y-1} \, dt
\]  

(5.38)
for $\text{Re}(x), \text{Re}(y) > 0$. It has the following striking evaluation, often established by using polar coordinates and double integrals (we shall see a third approach in the next section):

$$\beta(x, y) = \frac{\Gamma(x) \Gamma(y)}{\Gamma(x + y)}.$$  \hspace{1cm} (5.39)

This we shall now deduce from the Bohr-Mollerup result. We define $f = x \rightarrow \beta(x, y) \frac{\Gamma(x + y)}{\Gamma(y)}$ and proceed to verify the three properties. Point one is an easy integration exercise. For point two, we need to show $(1 + t/s)\beta(s + 1, t) = \beta(s, t)$. We observe that $\beta(s, t + 1) = \beta(s, t) - \beta(s + 1, t)$ which we combine with $\beta(s + 1, t) = (s/t)\beta(s, t + 1)$. It remains to show $f$ is log-convex as again follows by an application of Hölder’s inequality. Thus $f = \Gamma$ as required. In particular, we now obtain the famous evaluation

$$\Gamma \left( \frac{1}{2} \right) = \sqrt{\beta \left( \frac{1}{2}, \frac{1}{2} \right)} = \sqrt{\pi},$$ \hspace{1cm} (5.40)

as follows on making the change of variables $t = \cos(s)^2$ in the definition of the $\beta$–function. In the next subsection we shall link this formula to the volumes of $p$–balls in $\mathbb{R}^n$. \hfill \Box

The power of this approach is that it provides a generally applicable paradigm and that all or most can be automated or checked computationally—even when the general case may prove too hard to program, special cases can be checked symbolically or numerically, and add security! A second illustration is:

**Example 5.45.** The $\Gamma$–duplication formula.

$$\Gamma(2s) = 2^{2s-1} \Gamma(s) \Gamma(s + 1/2)/\sqrt{\pi}.$$  

This is established in the same way by considering

$$f(s) = \sqrt{\pi} \Gamma(2s)/(2^{2s-1} \Gamma(s + 1/2)).$$

In this case log-convexity has already been established and the other steps are easy in light of (5.40).

To complete this section, we derive the classical product for the sine function and relate it to the $\Gamma$–function. \hfill \Box

**Example 5.46.** The sin-product formula.

$$\sin(\pi x) = \pi x \prod_{n=1}^{\infty} \left( 1 - \frac{x^2}{n^2} \right)$$ \hspace{1cm} (5.41)
and
\[
\frac{\pi}{\sin(\pi x)} = \Gamma(x)\Gamma(1 - x). \tag{5.42}
\]

Now (5.42) follows directly from (5.41) and (5.36). We outline a proof of (5.41) whose full details are in [185]. We examine the polynomial
\[
P_m(x) = \frac{1}{2i} \left[ \left(1 + \pi i \frac{x}{m} \right)^m - \left(1 - \pi i \frac{x}{m} \right)^m \right] \to_m \sin(\pi x),
\]
and check that the roots of \(P_{2m}\) are 0, \(\pm (2k/\pi) \tan(j\pi/(2k))\) for \(0 < j < k\).

As the coefficient of \(x\) in \(P_{2m}\) is \(\pi\), we may write
\[
P_{2m}(x) = x \prod_{j=1}^{k-1} \left(1 - \frac{\pi^2 x^2}{4k^2 \tan^2(j\pi/(2k))}\right). \tag{5.43}
\]

Finally, one must take care to legitimate the passage to the limit in (5.43), using the fact that \(\tan(x)/x \to 1\) as \(x \to 0\).

One may heuristically derive (5.41) as Euler did by considering \(\sin(\pi x)\) as an “infinite” polynomial and rewriting it as a product in terms of the roots 0, \(\{1/n^2\}\). It is thus plausible that
\[
\frac{\sin(\pi x)}{x} = c \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2}\right), \tag{5.44}
\]
and Euler argues that as with a polynomial, \(c\) should be the value at zero and the coefficient of the linear term (in \(x^2\)) should be the sum of the roots: \(\sum_n n^{-2} = \pi^2/6\). The argument above made this both less obvious and more rigorous. Also, we emphasize that each step may be checked or discovered formally in many computer algebra packages.

### 5.4.1 Volumes of Balls

The volume of the unit ball in the \(\| \cdot \|_p\)-norm, \(V_n(p)\), was first determined by Dirichlet by explicitly evaluating the iterated integrals. He obtained
\[
V_n(p) = 2^n \frac{\Gamma(1 + \frac{1}{p})^n}{\Gamma(1 + \frac{2}{p})}, \tag{5.45}
\]
([5], Section 1.8). We note that the \(\Gamma\)-function again proves invaluable, and that even the special case when \(p = 2\),
\[
V_n = 2^n \frac{\Gamma(\frac{3}{2})^n}{\Gamma(1 + \frac{3}{2})} = \frac{\Gamma(\frac{3}{2})^n}{\Gamma(1 + \frac{3}{2})},
\]
gives a formula more concise than that recorded in most analysis books. One can try graphing this as a function of $p$ for $n = 2, 3, \ldots$, and observing the limiting cases $p = 1, \infty$.

The following Maple code derives this formula as an iterated integral for arbitrary $p$ and fixed $n$. The intermediate steps again give beta function values. The code can easily be converted into a human proof valid for arbitrary $n$.

```maple
vol := proc(n)
    local f, x, ul, u, j, t; global p;
    p := evaln(p);
    if n = 1 then 2 else
        f := (1 - add(x[i]^p, i = 1..n-1))^(1/p);
        for i from n-1 by -1 to 1 do
            f := subs(x[i]=t, f);
            f := int(f, t);
            ul := 1 - add(x[j]^p, j = 1..i-1);
            u := ul^(1/p);
            f := subs(t^p=ul, f);
            f := subs(t=u, f);
            f := map(normal, f);
            f := simplify(f);
        od;
        2^n*f;
    fi;
end:
```

It is also fun to determine in which dimension the volume of the Euclidean ball is maximized.

Let us recall the Laplace transform of a function $f$ defined by

$$
L(z) = L(f)(z) = \int_{0}^{\infty} e^{-zt} f(t) \, dt
$$

for $\text{Re}(z) > 0$. We finish the section with another, induction-free, Laplace transform-based, proof of (5.45). We shall evaluate

$$
v_p(y) = \text{Vol}_n(\{x : \|x\|_p \leq y\}),
$$

for $y > 0$ as follows. First, observe that

$$
v_p(y) = v_p(1) y^{n/p}.
$$

We now compute

$$
L(v_p)(1) = v_p(1) L(y \mapsto y^{n/p})(1) = v_p(1) \Gamma \left(1 + \frac{n}{p}\right). \tag{5.46}
$$
5.5 Stirling’s Formula

To evaluate the left-hand side we write

\[ L(v_p)(1) = \int_0^\infty e^{-t} \left( \int_{\|x\|_p \leq t} dx \right) dt = \int_\mathbb{R} \left( \int_0^\infty e^{-t} dt \right) dx = \int_\mathbb{R} e^{-\|x\|_p} dx = \prod_{k=1}^n \int_\mathbb{R} e^{-|x_k|^p} dx_k = 2^n \Gamma \left( 1 + \frac{1}{p} \right)^n. \tag{5.47} \]

Now comparing (5.46) and (5.47) recovers

\[ v_p(1) = 2^n \frac{\Gamma(1 + \frac{1}{p})^n}{\Gamma(1 + \frac{2}{p})} \]

as claimed. Moreover, most if not all of this can be performed by a good computer algebra integral transform package.

5.5 Stirling’s Formula

One of the most fundamental asymptotic formula in analysis is the so-called Stirling’s formula (actually due to De Moivre) for the factorial, and more generally, for the $\Gamma$ function.

**Theorem 5.47.**

\[ \lim_{n \to \infty} \frac{n!}{\sqrt{2\pi n} (n/e)^n} = 1 \tag{5.48} \]

and moreover, for $n > 1$

\[ 1 + \frac{1}{12n + 12} < \frac{n!}{\sqrt{2\pi n} (n/e)^n} < 1 + \frac{1}{12n - 24}. \tag{5.49} \]

While (5.48) yields an excellent relative error formula, (5.49) shows that the absolute error will be large. For example, with $n = 100$, the ratio is approximately $0.9997$, but the absolute error of the order of $10^{155}$. With more work, (5.49) can be made significantly more precise, but the version given is often more than sufficient.
Proof. To deduce the estimate we consider \( \log n! \) and argue as follows. By the trapezoidal formula (see Section 7.4 of the second volume), we have

\[
n \log(n) - n + 1 = \sum_{k=1}^{n-1} \int_{k}^{k+1} \log(x) \, dx
\]

\[
= \frac{1}{2} \sum_{k=1}^{n-1} [\log(k) + \log(k+1)] + \frac{1}{12} \sum_{k=1}^{n} e_k^{-2}, \tag{5.50}
\]

where \( e_k \) lies in \([k,k+1]\). If we denote this last series by \( R_n \), it is easy to see by the comparison test that it converges to a finite number \( R \). We may rewrite (5.50) as

\[
\left( \frac{n+1}{2} \right) \log(n) - n - \log(n!) \to R - 1,
\]

or equivalently that \( r_n = n^{-n/2} \exp(n) n! \) converges to a limit \( r \), and so also

\[
\lim_{n \to \infty} \frac{r_n^2}{\Gamma(2n+1)} = \frac{\Gamma(n+1)^2}{\Gamma(2n+1)} \sqrt{2}. \tag{5.51}
\]

Squaring, and taking the limit, we obtain

\[
r^2 = 4 \prod_{k=1}^{\infty} \frac{4k^2}{4k^2 - 1} = 2\pi, \tag{5.52}
\]

where this last identity is one of Wallis’ famous formulae. It may be derived from Euler’s product formula for \( \pi \) (5.41) with \( x = 1/2 \), or by repeatedly integrating \( \int_{0}^{\pi/2} \sin^{2n}(t) \, dt \) by parts. This establishes (5.48).

Now with a little more care, one can obtain (5.49) by estimating that \( 1/12(n+1) < R - R_n \leq 1/12(n-1) \), and considering the first few terms of the Taylor series for \( \exp \).

A very important consequence, derived along the way, is that the central binomial coefficient \( \binom{2n}{n} \sim 4^n / \sqrt{n} \), and you may equally easily estimate other binomial coefficients such as \( \binom{3n}{n} \), of the form examined elsewhere in this book.

It is interesting to consider how to be led to the correct result. First, to see that \( (n/e)^n \sqrt{n} \) is the right estimate and then to discover that \( r = \sqrt{2\pi} \), especially given that the convergence is only \( O(1/n) \).
5.6 Derivative Methods of Evaluation

Another potent and concrete way of establishing an identity is by obtaining an appropriate differential equation. For example consider

\[
\begin{align*}
f(x) & = \left( \int_0^x e^{-s^2} \, ds \right)^2 \\
g(x) & = \int_0^1 \frac{\exp(-x^2(1+t^2))}{1+t^2} \, dt.
\end{align*}
\]

The derivative of \( f + g \) is zero: In Maple,

```maple
f:=x->Int(exp(-s^2),s=0..x)^2;
g:=x->Int(exp(-x^2*(1+t^2))/(1+t^2),t=0..1);
with(student):d:=changevar(s=x*t,diff(f(x),x),t)+diff(g(x),x);
d:=expand(d);
```

shows this. Hence, \( f(s) + g(s) \) is constant for \( 0 \leq s \leq \infty \) and so, on justifying the limit at \( \infty \),

\[
\left( \int_0^\infty \exp(-t^2) \, dt \right)^2 = f(\infty) = g(0) = \arctan(1) = \frac{\pi}{4}.
\]

The change of variables \( t^2 = x \) shows that this evaluation of the normal distribution agrees with \( \Gamma(1/2) = \sqrt{\pi} \).

In similar fashion, we may evaluate

\[
F(y) = \int_0^\infty \exp(-x^2) \cos(2xy) \, dx
\]

by checking that it satisfies the differential equation \( F'(y) + 2y F(y) = 0 \). We obtain

\[
F(y) = \frac{\sqrt{\pi}}{2} \exp(-y^2),
\]

since we have just evaluated \( F(0) = \sqrt{\pi}/2 \), and again this is all easily implementable.

5.6.1 Legendre's Relation and Applications

We now turn to a study of the complete elliptic integral of the first and second kinds.
\[ K(k) = \int_0^{\pi/2} \frac{1}{\sqrt{1 - k^2 \sin^2(s)}} \, ds \]

\[ E(k) = \int_0^{\pi/2} \frac{\sqrt{1 - k^2 \sin^2(s)}}{\sqrt{1 - k^2}} \, ds \quad (5.53) \]

for \( k \) in \([0, 1]\).

We denote the complementary integrals by \( K'(k) = K(k') \), \( E'(k) = E(k') \) with \( k' = \sqrt{1 - k^2} \). A beautiful and important relationship follows:

**Theorem 5.48. (Legendre's Relation).** For all \( 0 < k < 1 \),

\[ E(k) K(k') + K(k) E'(k) - K(k) K'(k) = \frac{\pi}{2}. \]

**Proof.** It is easy to check that \( K \) and \( E \) satisfy the coupled second order differential equation:

\[ \frac{dK(k)}{dk} = \frac{E(k) - (1 - k^2)K(k)}{k(1 - k^2)} \quad \frac{dE(k)}{dk} = \frac{E(k) - K(k)}{k}. \]

These allow us to check, by hand or computer, that

\[ f(k) = E(k) K'(k) + K(k) E'(k) - K(k) K'(k) \]

has derivative zero. It remains to determine the constant. The easiest way is to evaluate \( \lim_{t \to 0} f(t) \). We observe that \( K(0) = E(0) = \pi/2 \) with error of order \( k \), and that \( E'(0) = 1 \); since \( K'(k) \sim \log(4/k) \), we determine that

\[ \lim_{t \to 0} f(t) = \frac{\pi}{2} + \lim_{t \to 0} (K(t) - E(t))K'(t) = \frac{\pi}{2}. \]

Legendre, in a tour de force, actually determined the constant by evaluating the four quantities at the third singular value \( k_3 = (\sqrt{3} - 1)/\sqrt{8} \).

This is discussed in detail in [49].

In a similar manner, we next evaluate \( K(1/\sqrt{2}) \) and \( E(1/\sqrt{2}) \).
5.6. Derivative Methods of Evaluation

The changes of variables \((s \rightarrow t \rightarrow x \rightarrow u)\) given in this Maple code reduces to

\[
K \left( \frac{1}{\sqrt{2}} \right) = \frac{1}{2\sqrt{2}} \beta \left( \frac{1}{2}, \frac{1}{4} \right) = \frac{\sqrt{\pi} \Gamma \left( \frac{1}{4} \right)}{\sqrt{8} \Gamma \left( \frac{1}{4} \right)} = \frac{\Gamma^2 \left( \frac{1}{4} \right)}{4\sqrt{\pi}}.
\]

on using (5.39), (5.40) and (5.42). By combining similar computations with (5.53), we may deduce that

\[
E \left( \frac{1}{\sqrt{2}} \right) = \frac{4 \Gamma^2 \left( \frac{3}{4} \right) + \Gamma^2 \left( \frac{1}{4} \right)}{8\sqrt{\pi}}.
\]

5.6.2 The AGM Iteration

The arithmetic-mean of Gauss and Legendre has already been introduced in previous chapters. Our goal in this section is to establish the basic properties of the iteration. As we noted, Gauss’s specific discovery was that the reciprocal of the integral

\[
\frac{2}{\pi} \int_0^1 \frac{dt}{\sqrt{1 - t^4}} \tag{5.54}
\]

agreed numerically with the limit of the rapidly convergent arithmetic-mean iteration given by \(a_0 = 1, \ b_0 = \sqrt{2}\) and computing

\[
a_{n+1} = \frac{a_n + b_n}{2}, \quad b_{n+1} = \sqrt{a_n b_n}. \tag{5.55}
\]

Indeed, the sequences \(a_n, b_n\) have a common limit \(1.1981402347355922074\ldots\)

It is a nice exercise to show that for all positive initial values, the iteration converges quadratically to a shared limit which we denote \(M(a, b)\), see [49]. It was the genius of Gauss that saw the limit. The next result gives a proof especially suited to computer verification or discovery.

**Theorem 5.49.**

\[
\frac{\pi/2}{M(a, b)} = \int_0^{\pi/2} \frac{dt}{\sqrt{a^2 \cos^2(t) + b^2 \sin^2(t)}}. \tag{5.56}
\]

**Proof.** We first show that

\[
I(a, b) = \frac{\pi/2}{M(a, b)}
\]
satisfies
\[ I(a, b) = I(A(a, b), G(a, b)), \]  
(5.57)
where \( A(a, b) = (a + b)/2 \) and \( G(a, b) = \sqrt{ab} \). Once this is shown, we have
\[ I(a, b) = I(a_n, b_n) = \cdots = I(M(a, b), M(a, b)) = \frac{\pi/2}{M(a, b)}, \]
as required since \( I(c, c) = \pi/(2c) \), as it is easy to justify exchanging the limit and the integral.

To establish (5.57), consider the following Maple code.

```maple
assume(a>0,b>0):
J:=simplify(changevar(s=b*tan(t),I(a,b),s),symbolic);
J1:=changevar(u=(s-a*b/s)/2,J,u); lprint(%);
j:=4/(a^2+(u-(u^2+a*b)^(1/2))^2)^1/2/((u-(u^2+a*b)^(1/2))^2+b^2)^1/2*
(u-(u^2+a*b)^(1/2))^2/((u-(u^2+a*b)^(1/2))^2+a*b);
j0:=1/sqrt((A(a,b)^2+u^2)*(G(a,b)^2+u^2));

The code implements the change of variables \( s = b \tan(t) \) and \( u = (s - ab/s)/2 \). The most problematic step is the verification that the consequent integrand, \( j_0/j \), simplifies as required. This is achieved by a \textit{resultant} computation:

\[ S:=simplify((j0/j)^2,radical); \]
\[ p1 := R^2 - (u^2+a*b); \]
\[ p2 := subs((u^2+a*b)^1/2 = R, Zero - (numer(S) - denom(S))); \]
\[ \text{resultant}( p1,p2,R); \text{simplify(series(j/j0,u,8))}; \]

and for peace of mind, the series of \( j/j_0 \) can be computed!  

Placing together (5.54) and (5.56), we have succeeded in establishing the discovery of Gauss in the form
\[ M(\sqrt{2},1) = \sqrt{\frac{2}{\pi}} 1^2 \left( \frac{3}{4} \right) = 1.1981402347355922074399224922803238\ldots, \]
using five steps of the iteration.

It is also possible to discover the form of the substitution \( u = (s - ab/s)/2 \), by taking a general quadratic form and solving for the parameters.
5.6. Derivative Methods of Evaluation

5.6.3 Other Mean Iterations

Finally, the more general study of means \[49\] also provides many opportunities for experimentation and computation. Consider a mean iteration, in which we start with \(a_0 > 0\) and \(b_0 > 0\) and iterate the discrete dynamical system

\[
a_{n+1} = M(a_n, b_n), \quad b_{n+1} = N(a_n, b_n)
\]

for two strict means, that is \(a > b\) implies \(a > M(a, b) > b\). This is a Gaussian iteration. The limit exists and is denoted \((M \otimes N)(a, b)\), and exhibits quadratic convergence when the means are symmetric. The triumph of the AGM is that we identify quadratic convergence to an important nonelementary function.

As a second example, consider

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

While it is hard to guess the (linearly convergent) limit, once told that it is the logarithmic mean

\[
L(a, b) = \frac{a - b}{\log(a) - \log(b)},
\]

proof of this fact reduces to showing the identity

\[
L(a, b) = L\left(\frac{a + \sqrt{ab}}{2}, \frac{b + \sqrt{ab}}{2}\right). \quad (5.58)
\]

The following Maple code implements the iteration:

```maple
L:=proc(a,b,n) local k,c,d; c:=a;d:=b; for k to n do (c,d):=(M(c,d),M(d,c)) od; end;
```

Thus, a hundred iterates yields

\[
L(2., 1., 100.) = 1.442695040889634073599246810014976\ldots
\]

while

\[
L(2, 1) = 1.442695040889634073599246810018921\ldots
\]

which agree to 30 places.
This illustrates the invariance principle asserting that limit is the unique mean $f$ with $f(a_n, b_n) = f(a_{n+1}, b_{n+1})$. In this case the means are not symmetric and convergence is only linear.

Similarly, we met the Archimedian iteration in Chapter 3. In this language, it is due to Gauss, Pfaff, Schwab, and Borchardt in the 19th century and establishes that

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

converges to

$$B(a, b) = \frac{\sqrt{b^2 - a^2}}{\arccos(a/b)}$$

for $0 < a < b$, and to

$$B(a, b) = \frac{\sqrt{a^2 - b^2}}{\arccosh(a/b)}$$

for $0 < b < a$. Armed with the invariance principle, the reader or her computer should be able to prove this assertion, and to determine the (linear) rate of convergence.

5.6.4 Gregory and Euler

We conclude this section by providing computer-verifiable proofs of

$$\frac{\pi}{4} = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{2k-1} \quad (5.59)$$

and

$$\frac{\pi^2}{6} = \sum_{k=1}^{\infty} \frac{1}{k^2}. \quad (5.60)$$

For the former, consider

$$\cot(x) = \frac{\cot(x/2) - \cot(\pi/2 - x/2)}{2}$$

and then observe that a telescoping identity yields

$$2^{-n} \sum_{k=1}^{2^n-1} (-1)^k \cot \left( \frac{(2k+1)\pi}{2^n} \right) = 1.$$
Recall that \(2^n \tan(a/2^n) \to a\), as \(n \to \infty\).

As always, we need to justify taking limits. The justification follows from Tannery’s theorem (a form of dominated convergence) and we have proven Gregory’s formula (5.59). Similarly, check that

\[
\csc^2(x) = \frac{\csc^2(x/2) + \csc^2(\pi/2 + x/2)}{4},
\]

and that a telescoping sum yields

\[
2 \sum_{k=0}^{2^n-1} \csc^2 \left(\frac{(2k+1)\pi}{2^n+1}\right) = 1.
\]

Again, taking limits carefully establishes

\[
\frac{\pi^2}{8} = \sum_{k=1}^{\infty} \frac{1}{(2k-1)^2},
\]

which is equivalent to (5.60), on separating odd and even terms.

While the technical details are important, from our perspective it is more interesting that we can perform all the steps experimentally, and worry about their legitimacy at the end, once we “know the truth!”

5.7 Commentary and Additional Examples

1. **A 3-D maximum problem.** Determine the maximum of

\[
f : (x, y, z) \mapsto \frac{\sin(x)^2}{x} + \frac{\sin(y)^2}{y} + \frac{\sin(z)^2}{z}
\]

for nonnegative \(x + y + z = \pi\). [Taken from [105].]

Solution: The unique maximum can be seen numerically to be \(x = y = z = 1.047197551196597\ldots\), which is clearly \(\pi/3\), and by symmetry one does expect that \(x = y = z\). Then observe that for all variables in \([0, \pi/2]\), \(f\) is strictly concave and so the critical point is a strict maximum value of \(27/(4\pi)\). Otherwise we may assume \(x > \pi/2\) and \(0 < y, z \leq \pi/2\). Let \(g\) denote \(x \mapsto \sin(x)^2/x\). Hence, by monotonicity and concavity \(f(x, y, z) \leq g(\pi/2) + f(0, y, z) < g(\pi/2) + 2g(\pi/4) = 6/\pi < 27/(4\pi)\).
2. An infinite product formula for the Gamma function. Show that
\[ \Gamma(x) = e^{-\gamma x} \prod_{n=1}^{\infty} \frac{e^{x/n}}{1 + x/n}, \]
for \( x > 0 \). Hint: Use the definition of \( \gamma \) and the product obtained in the conclusion of the Bohr-Mollerup Theorem.

3. A radially invariant generalization of \( \arctan(1) \). For each positive integer \( n \),
\[ \int_{[0,1]^n} \frac{dx_1 \cdots dx_n}{(1 + x_1^2 + \cdots + x_n^2)^{(n+1)/2}} = \frac{\pi^{(n+1)/2}}{(n+1)^2 \Gamma(\frac{n+1}{2})}. \]
Reason: Let
\[ A = \int_{[0,1]^n} \frac{dx_1 \cdots dx_n}{(1 + x_1^2 + \cdots + x_n^2)^{(n+1)/2}}, \]
\[ J = \int_{(0,\infty)^n} \frac{dx_1 \cdots dx_n}{(1 + x_1^2 + \cdots + x_n^2)^{(n+1)/2}}. \]
Each variable is maximal in one \( n \)th of the \( n \)-dimensional hypercube. So symmetry and setting \( y_n = 1/x_n, y_j = x_j y_n \) for \( 1 \leq j \leq n-1 \) gives
\[ J = n \int_{0}^{\infty} \int_{[0,y_n]^{n-1}} \frac{dy_1 \cdots dy_n}{(1 + y_1^2 + \cdots + y_n^2)^{(n+1)/2}} = n \int_{0}^{\infty} \int_{[0,1]^{n-1}} \frac{dx_1 \cdots dx_n}{(1 + x_1^2 + \cdots + x_n^2)^{(n+1)/2}} + \]
\[ = n \int_{0}^{1} \int_{[0,y_n]^{n-1}} \frac{dy_1 \cdots dy_n}{(1 + y_1^2 + \cdots + y_n^2)^{(n+1)/2}} = (n+1)A. \]
Thus
\[ A = \frac{J}{n+1} = \frac{1}{(n+1)^2} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \frac{dy_1 \cdots dy_n}{(1 + y_1^2 + \cdots + y_n^2)^{(n+1)/2}}. \]
We may now apply a standard result for radially invariant integrals over $\mathbb{R}^n$, in which we denote the surface measure of the unit $n$-sphere by $\sigma(S^{n-1}) = 2\pi^{n/2}/\Gamma(n/2)$. We have

\[
\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \frac{dy_1 \cdots dy_n}{(1 + y_1^2 + \cdots + y_n^2)^{(n+1)/2}} = \sigma(S^{n-1}) \int_{0}^{\infty} \frac{r^{n-1}}{(1 + r^2)^{(n+1)/2}} dr, \\
= \frac{\pi^{n/2}}{\Gamma(n/2)} \int_{0}^{\infty} \frac{u^{n/2-1}}{(1 + u)^{(n+1)/2}} du, \\
= \frac{\pi^{(n+1)/2}}{\Gamma((n + 1)/2)},
\]

via the beta integral, and the result follows.

4. The Psi function. Many sums can be expressed in terms of the $\Psi$ function and its derivatives, also known as polygamma functions. This is because

\[
\Psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} = \sum_{n=1}^{\infty} \frac{z}{n(z+n)} - \frac{1}{z} - \gamma,
\]

where the first equality is definitional.

(a) Show that $\Psi(1 + z) = \Psi(z) + 1/z$, that $\Psi(1) = -\gamma$, $\Psi(1/2) = -\gamma - 2 \log 2$, and $\Psi(n) = \sum_{k=1}^{\infty} 1/k - \gamma$. Obtain a similar formula for $\Psi(n + 1/2)$, for $n \in \mathbb{N}$.

(b) Prove that

\[
\Psi(z) - \Psi(1 - z) = \pi \cot (\pi z).
\]

(c) Obtain a duplication formula for $\Psi$ from that of $\Gamma$.

(d) Show that

\[
\Psi(z) = \int_{0}^{\infty} \frac{e^{-t} - e^{-zt}}{1 - e^{-t}} dt - \gamma
\]

and that for $n = 1, 2, 3, \ldots$

\[
\Psi^{(n)}(z) = (-1)^{n+1} \int_{0}^{\infty} \frac{t^n e^{-zt}}{1 - e^{-t}} dt
\]

for $\Re z > 0$. 
5. **Derangements.** A derangement is a permutation of \( n \) symbols that leaves no symbol in the same place. (a) Show that the number of derangements of \( n \) symbols, \( d_n \), satisfies the recursion
\[
d_n = (n - 1)d_{n-1} + (n - 1)d_{n-2}
\]
and has \( d_1 = 0, d_2 = 1 \). Hence, find (b) an exponential generating function \( E \), and (c) a closed form for \( d_n \).

Answer: (b) \[
\frac{\exp(-x)}{1 - x} = \sum_{k=1}^{\infty} \frac{d_k}{k!}.
\]
(c) Hence,
\[
d_n = n! \sum_{k=0}^{n} \frac{(-1)^k}{k!}.
\]

**Hint:** (a) Consider whether two objects are interchanged or not. (b) The differential equation satisfied by \( E \) is \( (1 - x)E' = xE \); now deduce (c). Alternatively, write \( d_n = n!b_n \) so that \( b_n - b_{n-1} = -(b_{n-1} - b_{n-2})/n \) and solve directly.

6. **An ODE pair.** Find a first order system of differential equations satisfied by
\[
a(x) = \int_{0}^{\infty} e^{-t} \frac{\sin (x \sqrt{t})}{\sqrt{t}} dt \quad (5.63)
\]
\[
b(x) = \int_{0}^{\infty} e^{-t} \frac{\cos (x \sqrt{t})}{\sqrt{t}} dt \quad (5.64)
\]
for \( x > 0 \) and so, or otherwise, solve for \( a \) and \( b \) explicitly. Answer:
\[
\sqrt{\frac{\pi (\sqrt{1 + x^2} \pm 1)}{2(1 + x^2)}},
\]
are the two functions.

7. **Maximum volume of unit ball.** Find the integer dimension \( N \) where the volume of the unit ball is maximized. For what real dimension is the volume maximized?

8. **A simple recursion.** Consider the recursion with \( a_0 = e, a_1 = 2e \) and
\[
n a_n = 2(a_{n-1} + a_{n-2}).
\]
5.7. Commentary and Additional Examples

Show that the ordinary generating function satisfies \( O' = 2(1 + x)O \), and thus \( O(x) = \exp((1 + x)^2) \). Hence, show

\[
a_{2n} = \sum_{m \geq 0} \frac{1}{(n + m)!} \binom{2n + 2m}{2n},
\]

and find a similar formula for the odd terms.

9. **Base-four sequences.** There are \( 4^n \) base-four sequence of length \( n \). How many are there with an odd number of zeroes? Answer: There are \( 2^n - 1 \) such sequences. *Hint:* The number is

\[
\sum \frac{1}{m_0!m_1!m_2!m_3!}
\]

summed over all partitions of \( n = m_0 + m_1 + m_2 + m_3 \) with \( m_0 \) odd. The exponential generating function is \( E(x) = \sinh(x)(\exp(x))^3 \).

10. **Putnam problem 1997–B5.** Let \( \tau_0 = 1 \) and \( \tau_n = 2^{\tau_{n-1}} \), for \( n \geq 1 \). Show that \( \tau_n \equiv \tau_{n-1} \mod n \). *Hint:* First, try some examples using *Maple* or *Mathematica*. Then use Fermat’s little theorem to show inductively the stronger claim that \( \tau_m \equiv \tau_{n-1} \mod n \) for \( m \geq n - 1 \).

11. **An integral identity.** Show that under very general conditions on \( f \), the identity

\[
\int_{-\infty}^{\infty} f(x)dx = \int_{-\infty}^{\infty} f(x - 1/x)dx
\]

holds. Use this to prove

\[
\int_{-\infty}^{\infty} e^{-x^2 - 1/x^2} dx = \frac{\sqrt{\pi}}{e^2}.
\]

12. **Berkeley problem 3.2.3.** Solve the differential equation

\[
\frac{d^2}{dx^2} y(x) - 2 \frac{d}{dx} y(x) + y(x) = \sin(x)
\]

with initial conditions \( y(0) = 1 \) and \( y'(0) = 0 \). *Hint:* Both *Maple* and *Mathematica* can solve this directly. Answer: \( y(x) = (1/2)e^x - (1/2)x e^x + (1/2) \cos(x) \).
13. A dilogarithm identity. The dilogarithm is a natural extension of $-\log(1 - x)$ defined by

$$\text{Li}_2(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^2}. $$

Prove, by differentiation, the functional equation

$$\text{Li}_2(x) + \text{Li}_2(1-x) - \log(x) \log(1-x) = \frac{\pi^2}{6}. $$

Hence, show

$$\text{Li}_2\left(\frac{1}{2}\right) = \sum_{n=1}^{\infty} \frac{1}{2^n n^2} = \frac{\pi^2}{12} - \frac{1}{2} \log^2(2). $$

There is a corresponding functional equation for the trilogarithm $\text{Li}_3(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^3}$. The functional equation developed by Landen around 1760 is

$$\text{Li}_3(x) + \text{Li}_3(1-x) + \text{Li}_3\left(\frac{x}{1+x}\right) = \zeta(3) + \zeta(2) \log(1-x) - \frac{1}{2} \log^2(1-x) \log(x) + \frac{1}{6} \log^3(1-x),$$

from which one can obtain closed forms at $x = 1/2$ and also at $x = (\sqrt{3} - 5)/2$ (see (5.65)).

14. Forensic mathematics. Lewin [141, 6.3.3] gives as (6.13) the identity

$$\text{Li}_3\left(\frac{3 - \sqrt{5}}{2}\right) = \frac{4}{5} \text{Li}_3(1) + \frac{\pi^2}{15} \log\left(\frac{3 - \sqrt{5}}{2}\right) - \frac{1}{12} \log^3\left(\frac{3\sqrt{5}}{2}\right)$$

(5.65)
due to Landen (1780), and then writes

These calculations are given in Edward’s Treatise on the Integral Calculus, Vol. 2, and there is quoted from Landen’s memoirs the equation

$$\frac{1}{1^3} + \frac{1}{2^3} + \frac{1}{3^3} + \cdots = \theta^3 + \frac{\theta^4}{2^3} + \frac{\theta^6}{3^3} + \cdots, \text{ where } \theta = 2 \sin(\pi/10).$$

This result is obviously incorrect, since the terms on the right are all less than the corresponding terms on the left, but a search
through the memoirs has failed to reveal any relation of the above type apart from the trivial one in which $\theta = 2 \sin(\pi/6)$, though it is difficult to believe this is the result which was intended. It might be pointed out that since $\theta^2 = (3 - \sqrt{5})/2$, such a relation between $Li_3(1)$ and $Li_3((3 - \sqrt{5})/2)$, if one should exist, would enable each to be isolated with the aid of (6.13), and there is no reason to expect that $Li_3(1)$ can in fact be calculated in this way. Edward's publishers have not succeeded in throwing any further light on the subject, and it looks as if this little mystery may have to remain unsolved.

The mystery remains. Can integer relation methods shed any new light?

15. Berkeley problem 6.10.7. Let $R$ be a commutative ring with a unit. Show that for all positive integers and all ring elements, the ideal generated by $a^n - 1$ and $a^m - 1$ is the same as that generated by $a^{[n,m]} - 1$. (Here $[n,m]$ denotes the gcd of $n$ and $m$). Hint: Let $n = sd$ and consider the factorization of $x^{sd} - 1$. Conversely, write $d = xn - ym$ and consider $a^d - 1 = (a^{xn} - 1) - a^d(a^{ym} - 1)$.

16. Berkeley problem 7.1.28. Let $\mathcal{P}$ denote all polynomials over $R$. Show that $p \mapsto p + p'$ is an invertible map on $\mathcal{P}$. Hint: Try low-degree polynomial examples.

17. Berkeley problem 7.5.23. Let $M_n^l$ be the $n \times n$ tridiagonal matrix with $a_{jj} = 2, a_{ij} = -1$ if $|i - j| = 1$ and all other entries zero. (a) Find the determinant of $M_n^l$ and (b) show that all eigenvalues are positive. Hint: Use Maple or Mathematica to find this determinant. Answer: (a) $\det(M_n^l) = n + 1$. (b) $M_n^l$ is positive definite.

18. Fibonacci and Lucas numbers in terms of hyperbolic functions. Show that $F_n$ is a constant times $i^{-n}\sinh(ns)$ and $L_n = 2i^{-n}\cosh(ns)$. Several formulas are then easy to obtain from the addition formulas for sinh and cosh.


20. Generalized arithmetic-geometric mean inequality. Show that the complex extension of the arithmetic-geometric mean inequality,

$$\left| \frac{a + b}{2} \right| \geq \sqrt{|ab|},$$
holds for complex \(a, b\) whose ratio \(a/b\) lies “outside” a certain cardioid in the complex plane. What can be found as a complex extension of 
\[
(a_1 + a_2 + \cdots + a_n)/n \geq (a_1a_2\cdots a_n)^{1/n}
\]
for positive \(a_1, a_2, \cdots a_n\)?

21. Viéte’s product.

\[
\frac{\sqrt{2}}{2} \frac{\sqrt{2 + \sqrt{2}}}{2} \frac{\sqrt{2 + \sqrt{2 + \sqrt{2}}}}{2} \cdots = \frac{2}{\pi}
\]

is considered to be the first truly infinite formula \[31\].

(a) Consider the following analogue of Viéte’s formula:

\[
P = \frac{\sqrt{2}}{\sqrt{1 + \sqrt{2}}} \frac{\sqrt{1 + \frac{\sqrt{2}}{\sqrt{1 + \sqrt{2}}}}}{\sqrt{1 + \frac{\sqrt{2}}{\sqrt{1 + \sqrt{2}}}}} \cdots .
\]

By writing a recursion for \(P\), determine the limit to high-precision and attempt to identify it. Then prove the conjectured result.

(b) Apply the same method to Viéte’s product.

(c) Consider \(t_0 = 0\) and \(t \mapsto (1 + \sqrt{3 - 2t})/2\).

**Hint:** (a) Consider the mapping \(t_0 = 1/\sqrt{2}\) and \(t \mapsto \sqrt{2/(1 + t)}\). (c) This should lead to a similar looking formula involving roots of two for \(2\sqrt{3}/\pi\). Answer: (a) \(K (1/\sqrt{2})/4\).

22. Berkeley problem 7.6.14. Show that a square Hermitian solution to \(A^5 + A^3 + A = 3I\) must be the identity. **Hint:** The minimal polynomial for \(A\) must have only real roots and divide \(t^5 + t^3 + t - 3\) which has one real root at 1.

23. Berkeley problem 7.9.16. Let

\[
A = \begin{bmatrix}
2 & -1 & 0 \\
-1 & 2 & -1 \\
0 & -1 & 2
\end{bmatrix}.
\]

Show that any matrix \(B\) that commutes with \(A\) must be a quadratic polynomial in \(A\). **Hint:** Consider the explicit form of a quadratic in \(A\) and the information implicit in \(AB - BA = 0\). This yields a set of linear equations that can be solved using Maple or Mathematica.
24. **Two proofs without words.** Show that
\[
\sum_{n=1}^{\infty} 2^n \frac{[1 - \cos (x/2^n)]^2}{\sin (x/2^{n-1})} = \tan \left( \frac{x}{2} \right) = \frac{x}{2}, \ |x| < \pi
\]
and
\[
2 \sum_{n=1}^{\infty} \frac{1 - \cos (x/2^n)}{\sin (x/2^{n-1})} = \tan \left( \frac{x}{2} \right), \ |x| < \pi.
\]
These arose from dissecting a kite (recursively) into a circular sector and triangles [67].

25. **From Ramanujan’s lost notebook.** The following examples appeared in Ramanujan’s lost notebook [35]:

(a) For \( t \geq 0 \) and \( a > 0 \), evaluate
\[
I(a, t) = \int_{-t}^{\infty} \frac{a^x}{\Gamma(x + 1)} dx + \int_{0}^{\infty} \frac{e^{-a x} x^{t-1}}{\pi^2 + \log^2 (x)} \left( \cos (\pi t) - \frac{\sin (\pi t)}{\pi} \log (x) \right) dx.
\]
(b) Hence, for \( s \geq 0 \), evaluate
\[
J(s) = \int_{0}^{\infty} \frac{s^x}{\Gamma(x + 1)} dx + \int_{0}^{\infty} \frac{e^{-s x}}{x (\pi^2 + \log^2 (x))} dx = I(s, 0).
\]
(c) For \( t \geq 0 \) and \( a > 0 \), evaluate
\[
K(a, t) = \int_{-t}^{\infty} \frac{a^x}{\Gamma(x + 1)} dx + \frac{\pi}{2} \int_{0}^{\infty} \left( \frac{e^{i \pi (t+ix)}}{a^{t+ix}} \Gamma(t+ix) + \frac{e^{-i \pi (t-ix)}}{a^{t-ix}} \Gamma(t-ix) \right) dx.
\]
(d) For \( a \geq 0 \) and \( 0 \leq \lambda < 1 \) evaluate
\[
\lim_{\epsilon \to 0} \epsilon \sum_{n=0}^{\infty} \frac{a^{(\lambda+n)\epsilon}}{\Gamma(1 + (\lambda + n)\epsilon)}.
\]

*Hint: (a) by differentiating \( I \) with respect to \( t \), show \( I(a, t) \) is a function of \( a \) alone. By differentiating \( I \) with respect to \( a \), identify the function up to a multiplicative constant. Evaluate \( I(0,0) \) to obtain the constant.*
(c) More elaborately, show $K(t, a)$ satisfies the same differential equation and finally, identify the constant by showing $K(1, 0) = J(1)$.

For (d), identify the limit as a Riemann integral.

Parts (a), (c) and (d) originate on pages 226 and 227 of the *Lost Notebook*, which was uncovered in Trinity College, Cambridge by George Andrews in 1976. Part (d) is a true part of a false “identity” in the notebook.

In a lecture entitled “25 years with Ramanujan’s Lost Notebook: Some General Observations” at the New York Academy of Sciences, Andrews, an Evan Pugh Professor of Mathematics at Pennsylvania State University, recalled the “heart-pounding excitement” of the moment when he realized he had come across a notebook detailing more than 135 pages of work from the last year in the life of the self-educated mathematical genius Ramanujan, the son of an accountant, who died at age 33 in 1920.

“That’s a moment that’s hard to beat,” Andrews said. “It was one of those great moments in life when for completely undeserved reasons you realize that you have stumbled across something that is extremely important.” In a talk that mixed Ramanujan’s biographical details with his mathematical theories, Andrews stressed the “surprise” that characterized the work of Ramanujan, a national hero in India. “Not many mathematicians are on postage stamps,” [Figure 3.2] he noted.

See [http://members.nyas.org/events/conference/mtg_02_1205.html](http://members.nyas.org/events/conference/mtg_02_1205.html).
Numerical Techniques

Far better an approximate answer to the right question, which is often vague, than the exact answer to the wrong question, which can always be made precise.


So far, we have focused on case studies of experimental mathematics in action. In this chapter, we will examine in more detail some of the underlying computational techniques that are used in this type of research. We will also mention a number of widely available tools for implementing these techniques, either commercially or freely via the Internet.

We shall discuss computational techniques such as high-precision arithmetic and integer relation detection, in part because these techniques are significantly more accessible than other aspects of experimental mathematics, such as symbolic computation. Further, the algorithms we describe here can be implemented in ordinary Java, C, C++, or Fortran-90 code. Such code can be enhanced for particular applications, potentially resulting in computer programs that out-perform commercial software for certain tasks. In contrast, symbolic computation requires some rather sophisticated techniques and data structures, and is thus not easily implemented by non-specialists. What’s more, advanced concepts, such as Groebner bases, are involved, which likely are unfamiliar to the majority of readers. As a result, we will, for the most part, not deal with symbolic computation here. Interested readers are referred to Joel Cohen’s newly published books on the topic [70, 71].

We focus here on practical algorithms and techniques. In some cases, there are known techniques that have superior efficiencies or other characteristics, but for various reasons are not considered suitable for practical implementation. We acknowledge the existence of such algorithms but do not, in most cases, devote space to them in these books.
6.1 Convolutions and Fourier Transforms

Convolutions and Fourier Transforms

Convolution computations frequently arise in experimental mathematics, in applications ranging from polynomial multiplication, which we will address in Chapter 14 of the second volume, to high-precision multiplication, which we will address in Section 6.2.4 and even the computation of the Riemann zeta function. The “acyclic” or “linear” convolution $A_k(x, y)$ of two $n$-long vectors $x = (x_n)$ and $y = (y_n)$ is defined as the $2n$-long vector

$$A_k(x, y) = \sum_{i+j=k} x_i y_j \quad 0 \leq k < 2n. \quad (6.1)$$

The cyclic convolution of $x$ and $y$ is defined as $n$-long vector

$$C_k(x, y) = \sum_{i+j=k} x_i y_j \quad 0 \leq k < n \quad (6.2)$$

$$= \sum_{j=0}^{n-1} x_j y_{k-j}, \quad (6.3)$$

where in this case the indices $i+j$ and $k-j$ are interpreted modulo $n$—i.e., $k-j$ is read as $k-j+n$ if $k-j < 0$.

For small values of $n$, these convolutions can be calculated explicitly as shown. For larger $n$ (typically $n \geq 64$ or so), significantly faster results can be obtained by employing fast Fourier transforms (FFTs). The FFT is merely an efficient means of computing the discrete Fourier transform (DFT) and the inverse discrete Fourier transform, which are defined for a complex sequence $z = (z_0, z_1, z_2, \cdots, z_{n-1})$ as follows:

$$F_k(z) = \sum_{j=0}^{n-1} z_j e^{-2\pi i j k / n} \quad 0 \leq k < n \quad (6.4)$$

$$F_k^{-1}(z) = \frac{1}{n} \sum_{j=0}^{n-1} z_j e^{2\pi i j k / n} \quad 0 \leq k < n.$$

An acyclic convolution can be reduced to a cyclic convolution simply by extending the $n$-long input vectors $x$ and $y$ to length $2n$ with zeroes. When this is done, we can write
6.1. Convolutions and Fourier Transforms

\[ A_k(x, y) = \sum_{j=0}^{2n-1} x_j x_{k-j}, \quad 0 \leq k < 2n, \tag{6.5} \]

where the subscript \( k-j \) is interpreted as \( k-j+2n \) when \( k-j < 0 \). Cyclic convolutions of size \( 2n \) can in turn be calculated using the DFT as

\[ c_k = F_k^{-1}[F_j(a)F_j(b)], \quad 0 \leq k < 2n. \tag{6.6} \]

The three DFTs indicated in the above formula, in turn, can be efficiently calculated by employing the FFT. The cost of an \( n \)-point FFT is roughly \( 5n \log_2 n \) operations, so the cost of three \( 2n \)-point FFTs is roughly \( 30n \log_2 n \). But in this case, where the input data vectors \( x \) and \( y \) are real, special variants of the FFT are widely known that reduce the computational cost to approximately half this figure, or roughly \( 15n \log_2 n \). These operation counts assume that \( n \) is a power of two, since the FFT algorithm is most efficient when \( n \) is a power of two.

We should note here that very efficient FFT library routines (even variants for real data input) are usually supplied by computer vendors as part of their scientific software libraries. There is also some excellent FFT software available from community software libraries, notably the FFTW software at [http://www.fftw.org](http://www.fftw.org). Thus it is usually not necessary for researchers to write their own FFT computation code. For those who do need to investigate further into FFT computation techniques, these are discussed in [11][190].

The DFT, as well as associated FFT computational techniques, are defined for finite-length sequences. As we have seen in Section 5.2, experimental mathematicians frequently encounter the continuous Fourier transform, which is defined for a real function \( f(t) \) on \( (-\infty, \infty) \) as

\[ \hat{f}(x) = \int_{-\infty}^{\infty} f(t)e^{-itx} \, dx \tag{6.7} \]

(see also Section 2.2 of the second volume). Discrete approximations to \( \hat{f}(x) \) can be found using the DFT and FFTs, as follows. Assume that \( f(t) \) is zero (or sufficiently small) outside the interval \([-a/2, a/2]\), and assume its Fourier transform \( \hat{f}(x) \) is zero (or sufficiently small) outside \([-b/2, b/2]\). Select an even integer \( n \) so that \( ab = 2\pi n \). The integer \( n \) is usually chosen to be a power of two, since this choice facilitates the usage of FFTs. A large value of \( n \) is often required to produce sufficient accuracy in the approximations below, so the parameters \( a \) and \( b \) may need to be increased.
to match the size of $n$. Given values of $a, b$, and $n$, we can write

$$\hat{f}\left(\frac{bk}{n}\right) = \int_{-\infty}^{\infty} f(t) e^{-itbk/n} dt$$

$$\approx \frac{a}{n} \sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} f\left(\frac{aj}{n}\right) e^{-i\left(\frac{aj}{n}\right)(bk/n)}$$

$$= \frac{a}{n} \sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} f\left(\frac{aj}{n}\right) e^{-2\pi ijk/n},$$

(6.8)

(6.9)

for $-n/2 + 1 \leq k \leq n/2$. If we adopt the convention that $f(t) = f(t - a)$ for $t > a/2$, and $\hat{f}(x) = \hat{f}(x - b)$ for $x > b/2$, then we can write

$$\hat{f}\left(\frac{bk}{n}\right) = \frac{a}{n} \sum_{j=0}^{n-1} f\left(\frac{aj}{n}\right) e^{-2\pi ijk/n},$$

(6.10)

for $0 \leq k \leq n - 1$, which is now in a form suitable for the application of FFTs.

An example of using this method to compute several Fourier transforms is given in Section 5.2.

### 6.2 High-Precision Arithmetic

We have already seen numerous examples of high-precision numerical calculations. Indeed, such computations frequently arise in experimental mathematics. We shall focus here on high-precision floating-point computation. High-precision integer computation is also required in some aspects of mathematical computation, particularly in prime number computations and symbolic manipulations, but as we shall see, many of the algorithms described below are equally applicable to both types of arithmetic. An excellent presentation of high-precision integer arithmetic is given in [77].

At this point in time, almost all computer systems support the IEEE-754 standard for floating-point arithmetic. The IEEE “single” (32-bit) format features roughly seven decimal digit accuracy and a dynamic range of $10^{\pm38}$. The IEEE “double” (64-bit) format features roughly 16 decimal digit accuracy and a dynamic range of $10^{\pm308}$. On many Intel and Intel-compatible processors, an additional “extended” (80-bit) format with roughly 19 digits is available. An IEEE “quad” (128-bit) format with roughly 33 decimal digits has been defined, but it is not yet implemented on any of the widely used microprocessors.
6.2. High-Precision Arithmetic

When higher precision arithmetic is required in experimental mathematics, many researchers employ the high-precision arithmetic facilities built into commercial software packages such as Maple and Mathematica. In both of these products, almost all defined functions can be numerically evaluated to arbitrarily high precision. One weakness of these products is that performance is significantly slower compared to what can be achieved using custom programs and libraries. However, intelligent usage of these custom libraries requires correspondingly greater understanding of the underlying nature of high-precision computation. Either way, some familiarity with this type of computation is essential.

6.2.1 Double-Double and Quad-Double Arithmetic

The most frequently needed form of high-precision arithmetic is twice that of the IEEE 64-bit format. As mentioned above, this level of precision is not yet widely available in hardware. However, it can be achieved by utilizing a pair of IEEE 64-bit “double” words, where the first word is the closest 64-bit word to the full value, and the second word is the difference (positive or negative) between the full value and the first word. Fortunately, this “double-double” arithmetic (with 106 mantissa bits or roughly 32 decimal digits) is both fast and easy to implement. This is due mainly to the thoughtful design of the IEEE floating-point standard, wherein the results of all arithmetic operations are guaranteed to be the closest possible value to the exact result for the given operands.

We briefly state here some key algorithms used in double-double arithmetic. Here ⊕, ⊖ and ⊗ denote the result of IEEE 64-bit arithmetic operations.

Algorithm 6.50. Double + double.

This computes the high- and low-order words of the sum of two IEEE 64-bit values $a$ and $b$.
1. $s := a \oplus b$;
2. $v := s \ominus a$;
3. $e := (a \ominus (s \ominus v)) \oplus (b \ominus v)$;
4. Return $(s, e)$.

Algorithm 6.51. Split.

This splits an IEEE 64-bit value $a$ into $a_{hi}$ and $a_{lo}$, each with 26 bits of significance and one hidden bit, such that $a = a_{hi} + a_{lo}$.
1. \( t := (2^{27} + 1) \otimes a; \)
2. \( a_{hi} := t \odot (t \odot a); \)
3. \( a_{lo} := a \ominus a_{hi}; \)
4. Return \((a_{hi}, a_{lo})\).

**Algorithm 6.52. Double \times double.**

This computes the high- and low-order words of the product of two IEEE 64-bit values \( a \) and \( b \).

1. \( p := a \otimes b \)
2. \((a_{hi}, a_{lo}) := \text{SPLIT}(a);\)
3. \((b_{hi}, b_{lo}) := \text{SPLIT}(b);\)
4. \( e := (((a_{hi} \odot b_{hi} \odot p) \oplus a_{hi} \odot b_{lo} \oplus a_{lo} \odot b_{hi}) \oplus a_{lo} \odot b_{lo});\)
5. Return \((p, e).\)

With regards to Algorithm 6.0, we should note that some processors, notably IBM PowerPC and RS6000 processors and Intel IA-64 processors, have a “fused multiply-add” instruction that greatly simplifies double \times double operations. In this case, one can simply write \( p := a \otimes b \) and \( e := a \odot b - p. \) Note, however, that it is often necessary to specify a special compiler option (such as -qstrict on IBM systems) to insure that this code is performed as written.

From these basic building blocks, one can construct a complete library of double-double arithmetic operations. For example, to add \((a_{1}, a_{2})\) to \((b_{1}, b_{2})\), it suffices to use Algorithm 6.0 to add \(a_{1}\) and \(b_{1}\), yielding high- and low-order results, then adding \(a_{2} + b_{2}\) to the low-order result. This scheme gives a double-double sum accurate to within two bits in the low-order word. A fully accurate result can be obtained with somewhat more effort. Double-double multiplication and division can be performed using straightforward adaptations of the classic multiplication and division schemes for decimal arithmetic. Full details are given in [116].

With somewhat more effort, “quad-double” arithmetic can be performed using these same methods. This features 212 mantissa bits or roughly 64 decimal digits. Note however that this arithmetic, like double-double arithmetic, does not extend the dynamic range, which remains roughly \(10^{\pm 308}\).

A software library implementing the above schemes is available on the Internet. This library, which is written in C, includes not only double-double but also quad-double routines. In addition to the basic arithmetic operations, many transcendental functions are also supported. Included in this package are C++ and Fortran-90 translation modules, which permit the library routines to be called from ordinary C++ and Fortran-90
6.2. High-Precision Arithmetic

Programs with only minor modifications to the source code, by utilizing operator overloading. Programs that use double-double arithmetic typically run five times slower than the equivalent 64-bit versions, and quad-double versions typically run 20 times slower. This software is available at http://www.experimentalmath.info

6.2.2 Arbitrary Precision Arithmetic

By “arbitrary precision” we mean a software facility that permits one to adjust the level of numeric precision over a wide range, typically extending to the equivalent of thousands or possibly even millions of decimal digits. An extended dynamic range is almost always included as well, since such computations often require a larger range than the \(10^{±308}\) range available with the IEEE double format.

For these levels of precision, the best approach is as follows. Define an arbitrary precision datum to be an \((n+4)\)-long string of words. The sign of the first word is the sign \(±\) of the datum, and the absolute value of the first word is \(n\), the number of mantissa words used. The second word contains an exponent \(p\). Words three through \(n+2\) are the \(n\) mantissa words \(m_i\), each of which has an integer value between 0 and \(2^b - 1\), or in other words \(b\) bits of the mantissa. Finally, words \(n+3\) and \(n+4\) are reserved as “scratch” words for various arithmetic routines. One can optionally designate an additional word, placed at the start of the data structure, to specify the amount of memory available for this datum, so as to avoid memory overwrite errors during execution. The value \(A\) represented by this datum is

\[
A = ±(2^{pb} m_1 + 2^{(p-1)b} m_2 + 2^{(p-2)b} m_3 + \cdots + 2^{(p-n+1)b} m_n),
\]

where it is assumed that \(m_1 \neq 0\) and \(m_n \neq 0\) for nonzero \(A\). Zero is represented by a string consisting of a sign word and an exponent word, both of which are zero.

There are several variations possible with this general design. One approach is to utilize 64-bit IEEE floating-point words, with \(b = 48\) mantissa bits per word. Addition operations can easily be performed by adding the two vectors of mantissas (suitably shifted to adjust for differences in exponent), and then releasing carries beginning from the last mantissa word back to the first. Multiplication and division can be performed by straightforward adaptations of the long multiplication and long division schemes taught in grammar school, performed modulo \(2^{48}\) instead of modulo 10. The multiplication of two individual 48-bit entities can be performed by 48-bit variations of Algorithms 6.0 and 6.0. In fact (and this is a key point for high performance), up to \(2^5 = 32\) such products can be accumulated
before needing to release carries, since $5 + 48 = 53$, and integers as large as $2^{53}$ can be accommodated exactly in a 64-bit IEEE word.

This approach was taken in the software package described in [26]. Like the double-double and quad-double libraries mentioned above, this software includes C++ and Fortran-90 translation modules, so that these functions can be invoked from ordinary programs with only minor modifications to the source code. The resulting software is available at the URL [http://www.experimentalmath.info](http://www.experimentalmath.info).

Another approach is to utilize arrays of integer data, with integer arithmetic operations, since all values in the data structure above are whole numbers. The disadvantage of this approach is that integer arithmetic is not as well standardized in microprocessors as floating-point arithmetic. Also, 64-bit integer multiplication is not yet universally supported in hardware. Thus it is hard to write programs that are both fast and easily portable to different systems. Nonetheless, some integer-based implementations have been successful, notably the GNU package, available at the URL [http://www.gnu.org/software/gmp/gmp.html](http://www.gnu.org/software/gmp/gmp.html).

### 6.2.3 Karatsuba Multiplication

One of the simplest schemes to accelerate multiprecision multiplication, and also one of the most widely used, was originally discovered by the Russian mathematician Karatsuba in 1962 [126]. It is based on the observation that if a high-precision number is split in two, then the full product can be obtained with only three half-sized times half-sized multiplications, instead of four as with conventional multiplication.

In particular, let $x$ be a number with $2b$-bit precision. We can write $x = x_0 + Bx_1$, where $B = 2^{-b}$ and $x_0$ and $x_1$ are binary fractions of comparable precision. Let $y$ similarly be represented as $y_0 + By_1$. Then we can compute as follows [77]:

\begin{align}
  t &= (x_0 + x_1) \cdot (y_0 + y_1) \\
  u &= (x_0 - x_1) \cdot (y_0 - y_1) \\
  v &= x_1 y_1 \\
  xy &= \frac{1}{2} (t + u) - v + \frac{B}{2} (t - u) + vB^2
\end{align}

Note that multiplications by $1/2$ and by $B$ are merely binary shifts of the “decimal” point. Thus the only expensive computations required here are the three multiplications involved in computing $t$, $u$, and $v$.

What’s more, this scheme can be applied recursively to perform the three indicated multiplications, until the multiplication problems are re-
6.2. High-Precision Arithmetic

Reduced to a size that ordinary grammar-school multiplication is preferred. It can be shown that the total number of operations in the recursive Karatsuba scheme is on the order of $(\log n)^{\log 3/\log 2}$, compared with $\log^2 n$ for classical schemes [77].

In practical implementations, the Karatsuba scheme is typically more economical than efficient conventional schemes beginning at roughly 400 decimal digit precision. It is not as efficient as FFT-based multiplication, which we will address in the next subsection (above roughly 1,000 decimal digit precision), but it is much easier to implement than a full-fledged FFT-based scheme. What’s more, it requires significantly less memory than a FFT-based scheme, for a given precision level. It is interesting to note that in several of Kanadas recent record-breaking computations of $\pi$, he used a Karatsuba scheme at the highest precision levels, and applied FFT-based schemes only when the Karatsuba recursion reached a certain precision level, where there was sufficient memory to use FFTs. For reasons such as these, the Karatsuba scheme is likely to remain a common fixture in high-precision computation packages.

6.2.4 FFT-Based Multiplication

The conventional and Karatsuba multiplication schemes are suitable for up to roughly 1000 decimal digit precision. For even higher levels of precision, significantly faster performance can be achieved by employing a convolution-FFT approach. Suppose we wish to multiply two $n$-precision values whose mantissa words (assuming a fixed number of bits per word) are given by $a = (a_0, a_1, a_2, \cdots, a_{n-1})$ and $b = (b_0, b_1, b_2, \cdots, b_{n-1})$. It is easy to see that the desired result, except for releasing carries, is simply the acyclic convolution of the $a$ and $b$ vectors, which can in turn be reduced to cyclic convolutions and then rapidly evaluated using FFTs.

This can be done as follows. First, extend the two vectors to length $2n$ by appending $n$ zeroes to each. Then the $2n$-long product $c$ of $a$ and $b$ is the cyclic convolution of $a$ and $b$:

$$c_k = \sum_{j=0}^{2n-1} a_j b_{k-j}, \quad 0 \leq k < 2n,$$

(6.15)

where by $b_{k-j}$ we mean $b_{k-j+2n}$ when $k-j$ is negative. This cyclic convolution is evaluated using FFTs as described earlier in the chapter. The $c_k$ results from the FFT process are floating-point numbers. Rounding these values to the nearest integer, and then releasing carries beginning at $c_{2n-1}$ gives the desired multiplication result.
One important issue here is that the FFT-based computation of the $c_k$ must be accurate enough to reliably recover their integer-valued results. For example, in a one million by one million decimal digit multiplication, the $c_k$ results are typically as large as $2^{113}$, and these must be reliably rounded to the correct integer values even in the presence of some floating-point roundoff error. A common solution is to split each input word containing 48 mantissa bits into 4 words, each containing 12 mantissa bits, and employ conventional 64-bit IEEE arithmetic in the FFT. The computational cost of this strategy is roughly $60n \log_2 n$ operations, where $n$ is the number of input words, but this is still much faster than conventional multiplication (roughly $30n^2$ operations, assuming Algorithms 6.0, 6.0, and 6.0) for higher levels of precision.

This scheme is suitable for precision levels up to approximately 10,000,000 decimal digits. As a precaution for computations above approximately 1,000,000 digits, it is wise to perform the following validity check: After rounding the results of the final inverse FFT to the nearest integer, also determine the largest difference between these results and the nearest integer. If this maximum difference is larger than, say, $3/8$, then the user should be alerted that the results can no longer be certified. To use the FFT-based approach for even higher levels of precision, it is necessary to divide the input data further, say to only 6 mantissa bits per 64-bit word, or to employ double-double arithmetic for the FFT. We might add that the test we describe above has also proven to be an effective computer system integrity test—one of the present authors has uncovered several flaws in computer hardware and software using this test.

Another detail worth mentioning here is that efficient FFTs are most commonly targeted to power-of-two data sizes. If your desired level of precision (measured in 64-bit words) is not a power of two, it is often possible to employ FFTs in the computation, yet avoid having to increase the precision level to the next highest power of two, which would double both the memory requirement and the computational cost. This can best be illustrated by example.

Consider the case $n = p + 2$, where $p = 2^r$ (so that $x_p, x_{p+1}, y_p$ and $y_{p+1}$ are potentially nonzero). First, extend the sequences $x$ and $y$ with zeroes to length $2p = 2^{r+1}$ (instead of length $2^{r+2}$ as in the conventional FFT procedure). Then apply forward and inverse FFTs to the extended sequences $x$ and $y$ to produce the circular convolution of these extended sequences, which is:

\[
\begin{align*}
  z_0 &= x_0y_0 + x_{p-1}y_{p+1} + x_py_p + x_{p+1}y_{p-1} \\
  z_1 &= x_0y_1 + x_1y_0 + x_py_{p+1} + x_{p+1}y_p
\end{align*}
\]
6.2. High-Precision Arithmetic

\[ z_2 = x_0y_2 + x_1y_1 + x_2y_0 + x_{p+1}y_{p+1} \]
\[ z_3 = x_0y_3 + x_1y_2 + x_2y_1 + x_3y_0 \]
\[ \cdots = \cdots \]
\[ z_p = x_0y_p + x_1y_{p-1} + \cdots + x_py_0 \]
\[ \cdots = \cdots \]
\[ z_{2p-1} = x_{p-2}y_{p+1} + x_{p-1}y_p + x_{p}y_{p-1} + x_{p+1}y_{p-2} \] (6.16)

This result differs from the desired \( 2^n \)-long linear convolution of \( x \) and \( y \) in two respects: (1) the initial three values \( (z_0, z_1, z_2) \) are “corrupted” with some additional terms, and (2) the final four members of the sequence are missing. These four missing values are

\[ z_{2n-4} = z_{2p} = x_{p-1}y_{p+1} + x_{p}y_p + x_{p+1}y_{p-1} \]
\[ z_{2n-3} = z_{2p+1} = x_{p}y_{p+1} + x_{p+1}y_{p} \]
\[ z_{2n-2} = z_{2p+2} = x_{p+1}y_{p+1} \]
\[ z_{2n-1} = z_{2p+3} = 0 \] (6.17)

Ignoring the last zero value, these three expressions are exactly the values that have “corrupted” the first three elements of the desired \( z \) sequence. Thus by separately computing these three expressions, one can correct the \( z \) sequence to the desired \( 2n \)-point linear convolution result. Note that these three values can be obtained by computing a linear convolution on the sequences \( \bar{x} = \{x_{p-1}, x_p, x_{p+1}\} \) and \( \bar{y} = \{y_{p-1}, y_p, y_{p+1}\} \) and discarding the first two elements of the six-long result. It is clear from this example that this technique can be extended to evaluate the linear convolution of sequences of size \( n = p + m \) for any \( m < p = 2^r \), although it is not efficient once \( m \) is larger than about \( 2^{r-1} \). The scheme can be applied recursively.

As it turns out, if one plots the computational cost (the number of arithmetic operations versus problem size) required for this scheme, the result is an intriguing fractal structure that is sometimes called the “devil’s staircase” (see Figure 6.1). For this reason, the above technique is sometimes referred to as the “devil’s convolution.” Additional details of this scheme are given in [14] [78].

Additional results and techniques for using various types of FFTs for high-precision arithmetic can be found in Crandall’s books on mathematical computation [78][77].

6.2.5 Algebraic and Transcendental Functions

So far we have focused on multiplication. In this section, we will describe some schemes for high-precision computation of several additional operations, including division and common transcendental functions. We present
here only an informal sketch of these methods. See [12, 26] for additional
details.

We start with a scheme for extra-high precision division. As we men-
tioned earlier, for moderate precision levels an adaptation of the conven-
tional grammar school division is adequate. Beyond several hundred digit
precision, it is faster to use a Newton iteration scheme, which involves only
multiplications, and a few other relatively inexpensive operations. Square
roots, cube roots and \( n \)-th roots for integers \( n > 3 \) can be found using
similar Newton iteration schemes.

Algorithm 6.53. **Extra-high precision division.**

To perform \( a/b \), first set \( x_0 \) to the 64-bit approximation of \( 1/b \), and then
employ a Newton iteration scheme to obtain \( 1/b \) to full precision:

\[
x_{k+1} = x_k + x_k(1 - bx_k).
\] (6.18)
6.2. High-Precision Arithmetic

Multiplying the final approximation to \(1/b\) by \(a\) gives the desired quotient. These iterations can be accelerated by utilizing a working precision level that approximately doubles with each iteration. Note that the above scheme involves only addition/subtraction operations and multiplies (which can be done using FFTs). If done carefully, the total computation cost is only slightly more than three times the cost of the final multiplication.

**Algorithm 6.54.** Square roots.

Square roots can be computed in a similar manner, using the Newton iteration for \(1/\sqrt{a}\):

\[
x_{k+1} = x_k + \frac{x_k}{2}(1 - ax_k^2).
\]

(6.19)

Multiplying the final approximation to \(1/\sqrt{a}\) by \(a\) gives the square root of \(a\). Some additional details are given in [26].

**Algorithm 6.55.** Pi.

The constant \(\pi\), which is needed for trigonometric functions, among other things, may be efficiently calculated using the Salamin-Brent algorithm: Set \(a_0 = 1\), \(b_0 = 1/\sqrt{2}\), and \(d_0 = \sqrt{2} - 1/2\). Then iterate the following arithmetic-geometric mean (AGM) operations beginning with \(k = 1\):

\[
a_k = \frac{(a_{k-1} + b_{k-1})}{2}, \quad b_k = \sqrt{a_{k-1}b_{k-1}}, \quad d_k = d_{k-1} - 2^k(a_k - b_k)^2.
\]

(6.20)

Then \(p_k = (a_k + b_k)^2/d_k\) converges quadratically to \(\pi\)—each iteration approximately doubles the number of correct digits. Unfortunately this algorithm is not self-correcting like algorithms based on Newton iterations. Thus all iterations must be done with at least the precision level desired for the final result.

The value of \(\pi\) can also be calculated quite rapidly using some of the infinite series presented in Chapter 3, for example Formulas (3.13), (3.14), or (3.19).

**Algorithm 6.56.** Exp.

For moderate levels of precision (up to roughly 1,000 decimal digits), \(e^t\) may be calculated using the following modification of the Taylor’s series for \(e^t\):

\[
e^t = \left(1 + r + \frac{r^2}{2!} + \frac{r^3}{3!} + \frac{r^4}{4!} \cdots\right) 256 \cdot 2^{2n},
\]

(6.21)
where \( r = t'/256 \), \( t' = t - n \log 2 \) and where \( n \) is chosen to minimize the absolute value of \( t' \). The exponentiation by 256 in this formula is performed by repeated squaring. Reducing \( t \) in this manner significantly accelerates convergence in the above series. On some systems, reducing by 1,024 instead of 256 is even faster.

**Algorithm 6.57. Log.**

Given this scheme for \( e^t \), moderate-precision natural logarithms of an argument \( a \) may then be calculated using the Newton iteration

\[
x_{k+1} = x_k + \frac{a - e^{x_k}}{e^{x_k}},
\]

using a doubling level of precision as before.

**Algorithm 6.58. Extra-high precision exp and log.**

For very high precision (beyond several hundred decimal digits), it is better to calculate logarithms by means of a quadratically convergent algorithm originally due to Salamin, as described by Brent in [57]. Inputs \( t \) that are extremely close to 1 are handled using a Taylor series. Otherwise, let \( n \) be the number of bits of precision required in the result. If \( t \) is exactly two, select \( m > n/2 \). Then the following formula gives \( \log 2 \) to the required precision:

\[
\log 2 = \frac{\pi}{2mA(1,4/2^m)}.
\]

Here \( A(a,b) \) is the limit of the AGM: Let \( a_0 = a \) and \( b_0 = b \), and iterate

\[
a_{k+1} = \frac{(a_k + b_k)/2}{b_{k+1}} = \sqrt{a_kb_k}
\]

until convergence. For other \( t \), select \( m \) such that \( s = t2^m > 2^n/2 \). Then the following formula gives \( \log t \) to the required precision:

\[
\log t = \frac{\pi}{2A(1,4/s)} - m \log 2.
\]

Given this scheme for logarithms, very high-precision exponentials can be calculated using Newton iterations, using a doubling level of precision as before.
6.3. Constant Recognition


For modest precision, one can calculate $\sin t$ via the Taylor’s series

$$\sin s = s - \frac{s^3}{3!} + \frac{s^5}{5!} - \frac{s^7}{7!} \cdots,$$  \hspace{1cm} (6.26)

where $s = t - a\pi/256$, and where the integer $a$ is chosen to minimize the absolute value of $s$. Then one calculates

$$\sin t = \sin(s + a\pi/256)$$
$$\cos t = \cos(s + a\pi/256),$$

by applying elementary trigonometric identities for sums. The required values $\sin(a\pi/256)$ and $\cos(a\pi/256)$ can be precalculated—they involve compound square roots of 2. Reducing $t$ in this manner significantly accelerates convergence in the above series for $\sin s$. On some systems, using 1,024 subdivisions instead of 256 is even faster. Inverse cosine and sine can then be calculated using Newton iterations.

Algorithm 6.60. Extra-high precision sin and cos.

For very high precision (above roughly 1,000 decimal digits), sines and cosines, as well as the inverse functions, can be calculated using complex arithmetic versions of the advanced algorithms described above for exp and log (recall that $e^{ix} = \cos x + i \sin x$). See [26] for full details.

An arbitrary precision software package implementing the above algorithms, including both basic arithmetic functions (with FFT-based schemes for very high precision) and numerous transcendental functions, is available from the URL [http://www.experimentalmath.info](http://www.experimentalmath.info).

6.3 Constant Recognition

Mathematicians have long dreamed of a facility that would recognize a computed numerical constant in an analytic formula in terms of known mathematical functions and constants. With some recent discoveries and algorithmic improvements, that day has arrived. Indeed, we have already seen numerous examples of this methodology in action. We describe here some of the algorithmic and numerical techniques involved.

Let $x = (x_1, x_2, \cdots, x_n)$ be a vector of real numbers. $x$ is said to possess an integer relation if there exist integers $a_i$, not all zero, such that
$a_1x_1 + a_2x_2 + \cdots + a_nx_n = 0$. By an integer relation algorithm, we mean a practical computational scheme that can recover the integers $a_i$, if they exist, or can produce bounds within which no integer relation exists.

Although the integer relation problem is often regarded to be a relatively “new” problem, it is really a rather old problem. The earliest reference is in the works of Euclid, whose Euclidean algorithm solves this problem in the case $n = 2$. A solution for $n > 2$ was attempted by numerous mathematicians in the 18th, 19th, and 20th centuries. The first general $n$ integer relation algorithm was discovered in 1977 by Ferguson and Forcade [93].

One approach to integer relation detection is to apply the Lenstra-Lenstra-Lovasz (LLL) lattice reduction algorithm. However, there are difficulties with this approach, notably the selection of a required multiplier—if it is too small, or too large, the LLL solution will not be the desired integer relation. Some of these difficulties were addressed in the “HJLS” algorithm [110], but this scheme suffers from numerical instability.

6.3.1 PSLQ

At the present time, the best integer relation algorithms are variants of the “PSLQ” algorithm [92], which was discovered in 1993 by Helaman Ferguson. PSLQ originally came to prominence with its role in the discovery of the BBP formula for $\pi$. In addition to possessing good numerical stability, PSLQ is guaranteed to find a relation in a polynomially bounded number of iterations. The name “PSLQ” derives from its usage of a partial sum of squares vector and a LQ (lower-diagonal-orthogonal) matrix factorization.

We present here a statement of the standard PSLQ algorithm. For additional details, see [92] [15] [23], from which this material has been adapted. Here $x$ is the $n$-long input real vector, and “nint” is the nearest integer function (for half-integer values, select the integer with greater absolute value). One selects the parameter $\gamma \geq \sqrt{4/3}$ (in our implementations, we select $\gamma = \sqrt{4/3}$).

**Algorithm 6.61. Standard PSLQ.**

Initialize:
1. Set the $n \times n$ matrices $A$ and $B$ to the identity.
2. For $k := 1$ to $n$ do: set $s_k := \sqrt{\sum_{j=k}^{n} x_j^2}$; enddo; set $t = 1/s_1$; for $k := 1$ to $n$ do: set $y_k := tx_k$; $s_k := ts_k$; enddo.
3. Compute the initial $n \times (n - 1)$ matrix $H$ as $H_{ij} = 0$ if $i < j$, $H_{jj} := s_{j+1}/s_j$, and $H_{ij} := -y_iy_j/(s_js_{j+1})$ if $i > j$. 
4. Reduce $H$: for $i := 2$ to $n$ do: for $j := i - 1$ to 1 step −1 do: set $t := \text{nint}(H_{ij}/H_{jj})$; and $y_j := y_j + ty_i$; for $k := 1$ to $j$ do: set $H_{ik} := H_{ik} - tH_{jk}$; enddo; for $k := 1$ to $n$ do: set $A_{ik} := A_{ik} - tA_{jk}$ and $B_{kj} := B_{kj} + tB_{ki}$; enddo; enddo; enddo.

Iterate the following until an entry of $y$ is within a reasonable tolerance of zero, or precision has been exhausted:
1. Select $m$ such that $\gamma_i|H_{ii}|$ is maximal when $i = m$.
2. Exchange the entries of $y$ indexed $m$ and $m+1$, the corresponding rows of $A$ and $H$, and the corresponding columns of $B$.
3. Remove the corner on $H$ diagonal: If $m \leq n - 2$ then set $t_0 := \sqrt{H_{mm}^2 + H_{m,m+1}^2}$, $t_1 := H_{mm}/t_0$ and $t_2 := H_{m,m+1}/t_0$; for $i := m$ to $n$ do: set $t_3 := H_{im}$, $t_4 := H_{i,m+1}$, $H_{im} := t_1 t_3 + t_2 t_4$ and $H_{i,m+1} := -t_2 t_3 + t_1 t_4$; enddo; endif.
4. Reduce $H$: for $i := m + 1$ to $n$ do: for $j := \text{min}(i - 1, m + 1)$ to 1 step −1 do: set $t := \text{nint}(H_{ij}/H_{jj})$ and $y_j := y_j + ty_i$; for $k := 1$ to $j$ do: set $H_{ik} := H_{ik} - tH_{jk}$; enddo; for $k := 1$ to $n$ do: set $A_{ik} := A_{ik} - tA_{jk}$ and $B_{kj} := B_{kj} + tB_{ki}$; enddo; enddo; enddo.
5. Norm bound: Compute $M := 1/\max_j |H_{jj}|$. Then there can exist no relation vector whose Euclidean norm is less than $M$.

Upon completion, the desired relation is found in the column of $B$ corresponding to the zero entry of $y$.

High-precision arithmetic must be used for almost all applications of PSLQ. In general, if one wishes to recover a relation of length $n$, with coefficients of maximum size $d$ digits, then the input vector $x$ must be specified to at least $nd$ digits, and one must employ floating-point arithmetic accurate to at least $nd$ digits. PSLQ typically recovers relations when the working precision is only 10 to 15 percent higher than this minimum value.

In the course of the operation of the PSLQ algorithm on a real computer system, the entries of the $y$ vector gradually decrease in size, with the largest and smallest entries usually differing by no more than two or three orders of magnitude. When a relation is detected by the algorithm, the smallest entry of the $y$ vector abruptly decreases to roughly the “epsilon” of the working precision (i.e., $10^{-p}$, where $p$ is the precision level in digits). The detection threshold in the termination test (iteration Step 6) above is typically set to be a few orders of magnitude greater than the epsilon value, in order to allow for reliable relation detection in the presence of some numerical roundoff error. The ratio between the smallest and the largest $y$ entry when a relation is detected can be taken as a “confidence level” that the relation is a true relation and not an artifact of insufficient numeric precision. Very small ratios at detection, such as $10^{-100}$, almost certainly
denote a true relation (although, of course, such results are experimental only, and do not constitute rigorous proof).

PSLQ runs reasonably fast for many problems, but in other cases large amounts of computer time are required. For these problems, one can utilize a two-level scheme, wherein most PSLQ iterations are performed using ordinary 64-bit IEEE double arithmetic, with the arbitrary-precision arrays updated as needed. This “two-level” scheme runs as much as 65 times faster on some problems. For very large problems, a three-level scheme yields further acceleration. Details of these methods are given in [23].

6.3.2 Multipair PSLQ

Even with the improvements mentioned above, PSLQ runtimes are painfully long for some very large problems of current interest. Thus one is led to consider employing modern parallel computer systems, which have the potential of many times faster performance than single-processor scientific workstations or personal computers.

Unfortunately, PSLQ, unlike most other algorithms used in experimental mathematics, is singularly unsuited for parallel computation. Large PSLQ calculations often require millions of iterations, each of which must be completed before the next begins. Furthermore, within an individual iteration, the key reduction operation (iteration Step 4) has a recursion that inhibits parallel execution, except at the innermost loop level. Thus there is virtually no concurrency to exploit in a parallel implementation.

Recently, a variant of the PSLQ algorithm, known as the “multipair” PSLQ algorithm, was discovered that dramatically reduces the number of sequential iterations, while at the same time exhibiting moderately high concurrency in the major steps of individual iterations. What’s more, it runs somewhat faster than the standard PSLQ even on single-processor systems.

Here $\gamma \geq \sqrt{4/3}$ and $\beta < 1/2$ are adjustable parameters (in our implementations, we set $\gamma = \sqrt{4/3}$ and $\beta = 2/5$).

**Algorithm 6.62.** Multipair PSLQ.

Initialize:
1. For $j := 1$ to $n$ do: for $i := 1$ to $n$ do: if $i = j$ then set $A_{ij} := 1$ and $B_{ij} := 1$ else set $A_{ij} := 0$ and $B_{ij} := 0$; enddo; enddo.
2. For $k := 1$ to $n$ do: set $s_k := \sqrt{\sum_{j=k}^{n} x_j^2}$; enddo; set $t = 1/s_1$; for $k := 1$ to $n$ do: set $y_k := tx_k$; $s_k := ts_k$; enddo.
3. Initial $H$: For $j := 1$ to $n - 1$ do: for $i := 1$ to $j - 1$ do: set $H_{ij} := 0$; enddo; set $H_{jj} := s_{j+1}/s_j$; for $i := j+1$ to $n$ do: set $H_{ij} := -y_j y_j/(s_j s_{j+1})$; enddo; enddo.

Iterate the following until an entry of $y$ is within a reasonable tolerance of zero, or precision has been exhausted:

1. Sort the entries of the $(n - 1)$-long vector $\{\gamma^i | H_{ii} | \}$ in decreasing order, producing the sort indices.

2. Beginning at the sort index $m_1$ corresponding to the largest $\gamma^i | H_{ii} |$, select pairs of indices $(m_i, m_i + 1)$, where $m_i$ is the sort index. If at any step either $m_i$ or $m_i + 1$ has already been selected, pass to the next index in the list. Continue until either $\beta n$ pairs have been selected, or the list is exhausted. Let $p$ denote the number of pairs actually selected in this manner.

3. For $i := 1$ to $p$ do: exchange the entries of $y$ indexed $m_i$ and $m_i + 1$, and the corresponding rows of $A$, $B$ and $H$; enddo.

4. Remove corners on $H$ diagonal: For $i := 1$ to $p$ do: if $m_i \leq n - 2$ then set $t_0 := \sqrt{H_{m_i,m_i}^2 + H_{m_i+1,m_i+1}^2}$; for $i := m_i$ to $n$ do: set $t_3 := H_{i,m_i}$; $t_4 := H_{i,m_i+1}$; $H_{i,m_i} := t_3 t_4 + t_4 t_3$; $H_{i,m_i+1} := -t_3 t_4 - t_4 t_3$; enddo; endif; enddo.

5. Reduce $H$: For $i := 2$ to $n$ do: for $j := 1$ to $n - i + 1$ do: set $l := i + j - 1$; for $k := j + 1$ to $l - 1$ do: set $H_{ij} := H_{ij} - T_{ik} H_{kj}$; enddo; set $T_{ij} := \text{nint}(H_{ij}/H_{jj})$ and $H_{ij} := H_{ij} - T_{ij} H_{jj}$; enddo; enddo.

6. Update $y$: For $j := 1$ to $n - 1$ do: for $i := j + 1$ to $n$ set $y_j := y_j + T_{ij} y_i$; enddo; enddo.

9. Update $A$ and $B$: For $k := 1$ to $n$ do: for $j := 1$ to $n - 1$: for $i := j + 1$ to $n$ do: set $A_{ik} := A_{ik} - T_{ij} A_{jk}$ and $B_{jk} := B_{jk} + T_{ij} B_{ik}$; enddo; enddo; enddo.

8. Norm bound: Compute $M := 1 / \max_{j} |H_{jj}|$. Then there can exist no relation vector whose Euclidean norm is less than $M$.

9. Termination test: If the largest entry of $A$ exceeds the level of numeric precision used, then precision is exhausted. If the smallest entry of the $y$ vector is less than the detection threshold, a relation has been detected and is given in the corresponding row of $B$.

There are several differences between this algorithm and the standard one-level PSLQ algorithm: (1) there is no reduction step in the initialization; (2) the $B$ matrix is transposed from the standard PSLQ algorithm; (3) up to $\beta n$ disjoint pairs (not just a single pair) of adjacent indices are selected in each iteration; (4) the $H$ reduction loop proceeds along successive lower diagonals of the $H$ matrix; (5) a $T$ matrix is employed, which contains the $t$ multipliers of the standard PSLQ; and (6) the $y$, $A$, and $B$ arrays are not updated with $H$, but in separate loops.
Unlike standard PSLQ, there is no proof that the multipair PSLQ scheme is guaranteed to find a relation within a polynomially bounded number of iterations. On the other hand, we have found, based on experience with a variety of sample problems, that the norm bound increases much more rapidly than in the standard PSLQ. Indeed, it appears that the selection of up to $\beta n$ disjoint pairs of indices in Step 2 above has the effect of reducing the iteration count by nearly the factor $\beta n$. This results in a significant saving in the number of expensive reduction and update steps.

The bottom line is that even on single processor systems, the multipair PSLQ algorithm appears to be significantly faster than the standard PSLQ \textsuperscript{23}. Both the standard PSLQ and the multipair PSLQ schemes, including two-level and even three-level variants, have been programmed in C++ and Fortran-90, targeted to the arbitrary precision package mentioned earlier in the chapter. This software is available from the URL [http://www.experimentalmath.info](http://www.experimentalmath.info).

### 6.3.3 Practical Constant Recognition

Practical constant recognition facilities require more than efficient integer relation detection schemes. Usually a sequence of methods are used. An approach that is used in some software is the following (here $\alpha$ is the input numerical constant) \textsuperscript{27}.

1. **Table look-up.** An indexed table of well-known numerical constants is checked to see if it contains $\alpha$, to within some tolerance.

2. **Algebraic check.** The vector $(1, \alpha, \alpha^2, \cdots, \alpha^n)$ is computed and then input to an integer relation finding routine, to see if $\alpha$ is an algebraic number of degree $n$ or less. The integer $n$ is chosen so that the runtime is reasonable for the numeric precision being used.

3. **Strided algebraic check.** The vector $(1, \alpha^{k}, \alpha^{2k}, \cdots, \alpha^{nk})$ is computed and then input to an integer relation finding routine, for integers $k$ up to some maximum level $m$. As before, the parameters $m$ and $n$ are selected to make runtimes reasonable.

4. **Multiplicative check.** $\log |\alpha|$ is computed, and then an integer relation check is done with the natural logarithms of the first few primes, as well as several other well-known constants, such as $\pi$, $e$, $\log 2$, $\log 3$, $G$ and $\gamma$ (here $G$ is Catalan’s constant and $\gamma$ is Euler’s gamma constant). If a relation is found in this set of numbers, then this means $\alpha$ is given by a one-term formula of the form

$$\alpha = \pm 2^a 3^b 5^c 7^d 11^e 13^f 17^g 19^h \pi^k e^l (\log 2)^m (\log 3)^n G^o \gamma^p$$
6.4 Commentary and Additional Examples

for rationals \(a, b, c, \cdots, p\). The number of primes and the set of other constants used here are quite arbitrary. They are typically chosen for effective constant discovery in a particular environment, under the constraint of reasonable run times.

5. Multiterm constant check. In this test, which is typically done with just double-double or with double precision, numerous integer relation tests are made for sample formulas that involve, for example, up to four terms, each of which has some combination of well-known mathematical constants. Thousands of such searches can be done in a few seconds. Such searches often turn up formulas that are not found using the above searches.

An online tool that employs this search strategy is available at the URL [http://www.cecm.sfu.ca/projects/ISC](http://www.cecm.sfu.ca/projects/ISC) A scheme employing a slightly different approach (a Java-based client) is available at [http://psg.cecm.sfu.ca/projects/revenge/client/RevEngClient.html](http://psg.cecm.sfu.ca/projects/revenge/client/RevEngClient.html). Software that performs this type of search strategy is also available as part of the Experimental Mathematician’s Toolkit: [http://wwwexperimentalmath.info](http://wwwexperimentalmath.info). Another interesting resource in this regard is Finch’s recently published *Mathematical Constants* [94].

Maple 9, released in summer 2003, incorporates a quite functional constant recognition tool. Typing `identify(3.146264370)` returns \(\frac{3}{2} + \frac{2}{2}\). One can expect such features with refinements in future releases of *Maple* and *Mathematica*.

6.4 Commentary and Additional Examples

1. **Continued fractions.** We should emphasize how continued fractions expose different structure: The golden mean is the simplest irrational, \(e\) shows great structure, \([1, 2, 3, 4, \cdots]\) is a ratio of Bessel functions, and \(\pi\) remains a complete mystery. Thus, a good rule in constant recognition is to always convert a decimal expansion to a simple continued fraction or to another base (say, binary), to see if this alternate representation is helpful.

2. **A new formula for Khintchine’s constant.** Let \(\{a_n\}\) be the continued fraction expansion of a random real number. The *Gauss-Kuz’min distribution* states that

\[
\text{Prob}(a_n = k) = -\log_2 \left[ 1 - \frac{1}{(k+1)^2} \right].
\]
Khintchine showed that, \( \lim_{k \to \infty} (a_1 a_2 \cdots a_k)^{1/k} \), the limiting geometric mean, exists a.e. and equals

\[
K_07 = \prod_{k=1}^{\infty} \left[ 1 + \frac{1}{k(k+2)} \right]^{\log_2 k} = \prod_{k=1}^{\infty} k^{\log_2 \left( 1 + \frac{1}{k} \right)}
\]

\[= 2.68545200106530644530971483548179569382038229399446 \ldots\]

Little is known about \( K_0 \). Is it rational, algebraic, or related to \( \pi \) or \( e \)? The formula is very slowly convergent.

For any positive integer \( N \), we may, however, derive a quite effective identity

\[
\log(K_0) \log(2) = \sum_{s=1}^{\infty} \zeta(2s, N) \frac{A_s}{s} - \sum_{k=2}^{N} \log \left( 1 - \frac{1}{k} \right) \log \left( 1 + \frac{1}{k} \right),
\]

where the Hurwicz zeta function is defined as

\[
\zeta(s, N) = \sum_{n=1}^{\infty} \frac{1}{(n+N)^s} = \zeta(s) - \sum_{n=1}^{N} n^{-s},
\]

while \( A_s = \sum_{k=1}^{2s-1} (-1)^{k-1}/k \) and \( N \) is a free parameter that can be varied for optimization and as an error check. The method has been used to compute \( K_0 \) to 7,350 digits—from which it seems to obey the Gauss-Kuz’min distribution [18].

3. **Putnam problem 1998–B5.** Let \( N \) be the “rep-one” integer consisting of 1,998 ones. Find the thousandth digit after the decimal point in \( \sqrt{N} \). Answer: The digit is a “1.” Hint: This can easily be verified by employing high-precision arithmetic. Once verified, this can be established by writing

\[
10^{1999} \sqrt{N} = \frac{\sqrt{10^{1999}} - 10^{2000}}{3},
\]

and so

\[
\frac{10^{1999} - 4}{3} < 10^{1999} \sqrt{N} < \frac{10^{1999} - 4}{3}.
\]

4. **Dynamical systems, numerical analysis, and formal power series.** We present here a brief overview of a surprising connection between numerical analysis of dynamical systems and formal power series [52]. We begin with a simple question: What, exactly, does the
fixed time step forward Euler numerical method do to the solution of the simple initial value problem
\[ \frac{dy}{dt} = y^2, \quad (6.27) \]
with \( y(0) = y_0 \). The numerical procedure is just
\[ y_{n+1} = y_n + hy'_n, \quad (6.28) \]
for integer \( n \geq 0 \), where \( y'_n = y_n^2 \) and \( h > 0 \) is the chosen time step.
It turns out to be useful to rescale \( y \) and \( t \) so that \( v = hy \) and \( \tau = ht \), giving
\[ \frac{dv}{d\tau} = v^2, \quad (6.29) \]
and (6.28) becomes
\[ v_{n+1} = v_n + v_n^2. \quad (6.30) \]
We may then rephrase our question to ask instead what the relation-
ship between \( v_n \) and \( v(\tau) \) is.
The point of view taken in [73] is that of backward error analysis.
That is, instead of asking for the difference between \( v(n) \) and \( v_n \), we
ask instead if there is another differential equation, say
\[ \frac{dw}{d\tau} = B(w)w^2, \quad (6.31) \]
whose solution interpolates \( v_n \). That is, we impose the conditions
\( w(0) = v_0 \) and \( w(\tau + 1) = w(\tau) + w(\tau)^2 \) (see Formula (6.30), and see
if we can find such a function \( B(w) \).
It turns out that we can use the method of modified equations [104] to
find as many terms of the Taylor series for \( B(w) \) as we desire. When
we compute the modified equation for (6.27) to (say) fifth order, we
get
\[ \frac{dw}{dt} = \left( 1 - w + \frac{3}{2!}w^2 - \frac{16}{3!}w^3 + \frac{124}{4!}w^4 - \frac{1256}{5!}w^5 \right) w^2. \quad (6.32) \]
Now we see the sequence 1, \(-1, 3, \frac{16}{2!}, \frac{124}{4!}, \frac{1256}{5!} \) appearing. This is
sequence M3024 in Sloane’s dictionary [182], which points us directly
to the very beautiful and useful paper [136]. It tells us that if
\[ B(w) = \sum_{n \geq 0} c_n w^n, \quad (6.33) \]
then
\[ c_n = \frac{1}{n-1} \sum_{i=1}^{n-1} \binom{n-i+1}{i+1} c_{n-i}, \]
and this, combined with the functional equation
\[ B(w) = \frac{(1 + w)^2}{1 + 2w} B(w + w^2) \]
(which can be iterated to give us two converging infinite products for \( B \)), allows us to write an efficient program to evaluate \( B(w) \). We can show that \( B(w) \) has a pole at \( w = -1/2 \); by mapping backwards, solving \( w + w^2 = -1/2 \), we find two more (complex) poles. Iterating this process finds an infinite number of complex poles, approaching the Julia set for the map \( v \rightarrow v + v^2 \) arbitrarily closely; see Figure 6.2.

The Julia set itself approaches the origin arbitrarily closely. That is, there are poles arbitrarily close to the point of expansion of the series given for \( B \). Thus the series (6.33) diverges—but, nonetheless, it can be used to evaluate \( B(w) \) for \( w \) close enough to zero, using the built-in sequence acceleration techniques of Maple. This is precisely where the convergent infinite products are slow, and hence, the series is useful. See [73] for details.

Figure 6.2. The first 16,000 poles of \( B(v) \), approaching the Julia set of \( v \rightarrow v + v^2 \).
5. **Accelerations for Catalan’s constant.** (This material is condensed from [56].) Acceleration formulas for slowly convergent series such as Catalan’s constant may be based on transformations of the log tangent integral. The simplest acceleration formula of its type is

\[
G = \frac{\pi}{8} \log(2 + \sqrt{3}) + \frac{3}{8} \sum_{k=0}^{\infty} \frac{1}{(2k + 1)^2 \binom{2k}{k}},
\]  

(6.34)
due to Ramanujan. This is the first of an infinite family of formulae for \( G \), each of which includes an infinite series whose general term consists of a linear recurrence damped by the summand in (6.34).

Each series evaluates to a rational linear combination of \( G \) and \( \pi \) times the logarithm of an algebraic unit (i.e., an invertible algebraic integer). The most striking example is

\[
G = \frac{\pi}{8} \log \left( \frac{10 + \sqrt{50 - 22\sqrt{5}}}{10 - \sqrt{50 - 22\sqrt{5}}} \right) + \frac{5}{8} \sum_{k=0}^{\infty} \frac{L_{2k+1}}{(2k + 1)^2 \binom{2k}{k}},
\]

(6.35)

where \( L_1 = 1, \ L_2 = 3, \) and \( L_n \) are the Lucas numbers (M0155 in Sloane’s Encyclopedia).

The series acceleration results (6.34) and (6.35) appear as natural consequences of transformation formulae for the log tangent integral, although Ramanujan apparently derived his result (6.34) by quite different methods. The connection with log tangent integrals is best explained by the equation

\[
G = -\int_{0}^{\pi/4} \log(\tan \theta) \, d\theta,
\]

(6.36)

obtained by expanding the integrand into its Fourier cosine series and integrating term by term. Ramanujan’s result (6.34) arises from the transformation

\[
2 \int_{0}^{\pi/4} \log(\tan \theta) \, d\theta = 3 \int_{0}^{\pi/12} \log(\tan \theta) \, d\theta.
\]

(6.37)

Formula (6.35) arises similarly from the transformation

\[
2 \int_{0}^{\pi/4} \log(\tan \theta) \, d\theta
= 5 \int_{0}^{3\pi/20} \log(\tan \theta) \, d\theta - 5 \int_{0}^{\pi/20} \log(\tan \theta) \, d\theta.
\]

(6.38)
A great virtue of such log tangent identities is that they can be efficiently hunted for by integer relation methods.

6. **More Catalan formulas.** Evaluate

(a) \[
\sum_{n \geq 1} \frac{n}{16^n} \zeta(2n + 1),
\]
due to Glaisher (1913), and

(b) \[
\sum_{n \geq 1} (n + 1) \frac{3^n - 1}{4^n} \zeta(n + 2),
\]
due to Flajolet and Vardi (1996) in terms of Catalan’s constant.

7. **Continued fraction for Euler’s constant.** Compute the simple continued fraction for Euler’s constant and see if it appears to satisfy the Gauss-Kuz’min distribution.

8. **The perceptual dipper effect.** Over the past decade, the JPEG image compression standard (see [http://www.jpeg.org](http://www.jpeg.org)) originally named for the Joint Photographic Experts Group, has become the benchmark for compressing natural still images for use on the internet. This standard has been extremely successful in maintaining a balance between low file size and high subjective image quality. However, JPEG-encoded images can exhibit unexpected objectionable artifacts. For example, for images already encoded using compression methods based around the discrete cosine transform (DCT), further compression by requantization can create objectionable visual artifacts. This phenomenon, called the JPEG perceptual dipper effect, is an example of the more general concept of a visual threshold, wherein two approximations of the same original image, which differ little from each other in terms of some given numerical measure, differ dramatically in the “quality” of their visual fidelity to the original image.

The dipper effect is illustrated in Figure 6.3. The mandrill image in the center is more compressed than the leftmost, yet appears better than the one on the left, and compares quite favorably to the much less compressed image on the right. The effect can be easily avoided by simple calculations in the process of designing the quantization matrices used to re-quantize the given image. This is of practical
consequence for delivery of images where bandwidth or storage is an issue (such as in delivery of data to cell phones, PDAs and other wireless devices), since it is possible to assess and exploit the dipper effect in software ([31] and [148]). Needless to say, such effects must be seen to be discovered.

9. **The Universal Computer: The road from Leibniz to Turing.**

This is an engaging account by Martin Davis of the history of logic and the birth of the modern computer [81]. In his story—chock full of colorful detail, such as Frege’s extreme antisemitism and Gödel’s conversion to full-blooded Platonism—one reads

(a) “For it is unworthy of excellent men to lose hours like slaves in the labor of calculation which could be safely relegated to anyone else if the machine were used.” (Leibniz)

(b) That Poincaré is reputed to have said Cantor’s set theory “would be regarded as a disease from which one had recovered.” and that he did write of Russell, “It is difficult to see that the word \( \uparrow \) acquires when written \( \supset \), a virtue it did not possess when written \( \uparrow \).”

(c) “To exist in mathematics means to be constructed by intuition; and the question whether a certain language is consistent, is not only unimportant in itself, it is also not a test for mathematical existence.” (Brouwer)

(d) That Hardy, of Hilbert’s *Entscheidungsproblem* (decision problem), said correctly, “There is of course no such Theorem and this is very fortunate, . . .”
(e) When Turing, after showing the unsolvability of the halting problem, went to Princeton to work with Church and others in 1936, von Neumann wrote him a letter of reference that made no mention of his work on computability (von Neumann reportedly said that after what Gödel did he would never read another paper in logic). But by the beginning of World War Two, von Neumann was openly using Turing’s ideas and goals of building practical computing machines. By the end of Turing’s wartime stay at Bletchley Park, he had played a key role in breaking the German codes and was in possession of “a working knowledge of vacuum electronics.”

The last chapters of [81] tell of the development of Turing’s computer science influenced Automatic Computing Machine (ACE) and von Neumann and others’ more engineering influenced ENIAC, about which Turing may have been thinking when he wrote of “the American tradition of solving one’s difficulties by much equipment rather than by thought.” By the end of the last century, Turing was recognized along with von Neumann as the intellectual progenitors of modern computing. Davis summarized his account with these words:

“This story underscores the power of ideas and the futility of predicting where they will lead.” (Martin Davis)
7 Making Sense of Experimental Mathematics

7.1 Introduction

Philosophers have frequently distinguished mathematics from the physical sciences. While the sciences were constrained to fit themselves via experimentation to the “real” world, mathematicians were allowed more or less free reign within the abstract world of the mind. This picture has served mathematicians well for the past few millennia but the computer has begun to change this. The computer has given us the ability to look at new and unimaginably vast worlds. It has created mathematical worlds that would have remained inaccessible to the unaided human mind, but this access has come at a price. Many of these worlds, at present, can only be known experimentally. The computer has allowed us to fly through the rarefied domains of hyperbolic spaces and examine more than a billion digits of \( \pi \) but experiencing a world and understanding it are two very different phenomena. Like it or not, the world of the mathematician is becoming experimentalized.

The computers of tomorrow promise even stranger worlds to explore. Today, however, most of these explorations into the mathematical wilderness remain isolated illustrations. Heuristic conventions, pictures and diagrams developing in one sub-field often have little content for another. In each sub-field unproven results proliferate but remain conjectures, strongly held beliefs or perhaps mere curiosities passed like folk tales across the Internet. The computer has provided extremely powerful computational and conceptual resources but it is only recently that mathematicians have begun to systematically exploit these abilities. It is our hope that by focusing on experimental mathematics today, we can develop a unifying methodology tomorrow.

\(^1\)This entire chapter is a reprint (with permission of Springer-Verlag) of “Making Sense of Experimental Mathematics,” by J. M. Borwein, P. B. Borwein, R. Girgensohn, and S. Parnes, *Mathematical Intelligencer*, vol. 18 (1996), page 12–18.
7.1.1 Our Goals

The genesis of this article was a simple question: “How can one use the computer in dealing with computationally approachable but otherwise intractable problems in mathematics?” We began our current exploration of experimental mathematics by examining a number of very long-standing conjectures and strongly held beliefs regarding decimal and continued fraction expansions of certain elementary constants. These questions are uniformly considered to be hopelessly intractable given present mathematical technology. Unified field theory or cancer’s “magic bullet” seem accessible by comparison. But like many of the most tantalizing problems in mathematics their statements are beguilingly simple. Since our experimental approach was unlikely to result in any new discoveries\footnote{We will not discuss the computational difficulties here but there are many non-trivial mathematical and computer-related issues involved in this project.}, we focused on two aspects of experimentation: systematization and communication.

For our attempted systematization of experimental mathematics we were concerned with producing data that were “completely” reliable and insights that could be quantified and effectively communicated. We initially took as our model experimental physics. We were particularly interested in how physicists verified their results and the efforts they took to guarantee the reliability of their data. The question of reliability is undoubtedly central to mathematicians and here we believe we can draw a useful distinction between experimental physics and mathematics. While it is clearly impossible to extract perfect experimental data from nature such is not the case with mathematics. Indeed, reliability of raw mathematical data is far from the most vexing issue.

Let us turn to our second and primary concern: insight. All experimental sciences turn on the intuitions and insights uncovered through modeling and the use of probabilistic, statistical and visual analysis. There is really no other way to proceed, but this process even when applied to mathematics inevitably leads to some considerable loss of exactness.

The communication of insight, whether derived from mathematical experiment or not, is a complex issue. Unlike most experimentalized fields, Mathematics does not have a “vocabulary” tailored to the transmission of condensed data and insight. As in most physics experiments the amount of raw data obtained from mathematical experiments is, in general, too large for anyone to grasp. The collected data needs to be compressed and compartmentalized. To make up for this lack of unifying vocabulary we have borrowed heavily from statistics and data analysis to interpret our results. For now we have used restraint in the presentation of our
7.1. Introduction

results in what we hope is an intuitive, friendly and convincing manner. Eventually what will probably be required is a multi-leveled hyper-textual presentation of mathematics, allowing mathematicians from diverse fields to quickly examine and interpret the results of others—without demanding the present level of specialist knowledge. [Not only do mathematicians have trouble communicating with lay audiences, but they have significant difficulty talking to each other. There are hundreds of distinct mathematical languages. The myth of a universal language of mathematics is just that. Many subdisciplines simply can not comprehend each other.]

7.1.2 Unifying Themes

We feel that many of these problems can be addressed through the development of a rigorous notion of experimental mathematics. In keeping with the positivist tradition, mathematics is viewed as the most exact of sciences and mathematicians have long taken pride in this. But as mathematics has expanded, many mathematicians have begun to feel constrained by the bonds placed upon us by our collective notion of proof. Mathematics has grown explosively during our century with many of the seminal developments in highly abstract seemingly non-computational areas. This was partly from taste and the power of abstraction but, we would argue, equally much from the lack of an alternative. Many intrinsically more concrete areas were, by 1900, explored to the limits of pre-computer mathematics. Highly computational, even “brute-force” methods were of necessity limited but the computer has changed all that. A re-concretization is now underway. The computer–assisted proofs of the four color theorem are a prime example of computer–dependent methodology and have been highly controversial despite the fact that such proofs are much more likely to be error free than, say, even the revised proof of Fermat’s Last Theorem.

Still, these computerized proofs need offer no insight. The Wilf/Zeilberger algorithms for “hypergeometric” summation and integration, if properly implemented, can rigorously prove very large classes of identities. In effect, the algorithms encapsulate parts of mathematics. The question raised is: “How can one make full use of these very powerful ideas?” Doron Zeilberger has expressed his ideas on experimental mathematics in a paper dealing with what he called “semi-rigorous” mathematics. While his ideas as presented are somewhat controversial, many of his ideas have a great deal of merit.

The last problem is perhaps the most surprising. As mathematics has continued to grow there has been a recognition that the age of the mathematical generalist is long over. What has not been so readily acknowledged is just how specialized mathematics has become. As we have already ob-
served, sub-fields of mathematics have become more and more isolated from each other. At some level, this isolation is inherent but it is imperative that communications between fields should be left as wide open as possible.

As fields mature, speciation occurs. The communication of sophisticated proofs will never transcend all boundaries since many boundaries mark true conceptual difficulties. But experimental mathematics, centering on the use of computers in mathematics, would seem to provide a common ground for the transmission of many insights. And this requires a common meta-language\(^3\). While such a language may develop largely independent of any conscious direction on the part of the mathematical community, some focused effort on the problems of today will result in fewer growing pains tomorrow.

7.2 Experimental Mathematics

7.2.1 Journal of

A professor of psychology was exploring the creative process and as one of his subjects chose a mathematician who was world famous for his ability to solve problems. They gave him a problem to work on. He wrote something down and immediately scribbled it out. He wrote something else down and scribbled it out. The professor asked him to leave everything on the page. He explained that he was interested in the process, the wrong answers and the right answers. The mathematician sat down. Wrote something. The psychology professor waited in anticipation but the mathematician announced he could not proceed without erasing his mistakes. While the mathematician in this situation is undoubtedly fairly idiosyncratic in how he attacks problems there is a strongly felt separation between the creative process of mathematics and the published or finished product.

A current focal point for experimental mathematics is the journal called *Experimental Mathematics*. But does it really seek to change the way we do mathematics, or to change the way we write mathematics? We begin by attempting to extract a definition of “experimental” from the Journal’s introductory article (\([87]\)) “About this Journal” by David Epstein, Silvio Levy and Rafael de la Llave.

The word “experimental” is conceived broadly: many mathematical experiments these days are carried out on computers, but others are still the result of pencil-and-paper work, and there are other experimental techniques, like building physical models. (\([87]\) p. 1)

\(^3\)This may not be a fanciful dream as the *Computer Algebra Systems* (CAS) of today are beginning to provide just that.
It seems that almost anything can be conceived of as being experimental. Let us try again.

Experiment has always been, and increasingly is, an important method of mathematical discovery. (Gauss declared that his way of arriving at mathematical truths was “through systematic experimentation”.) Yet this tends to be concealed by the tradition of presenting only elegant, well-rounded and rigorous results. ([87] p. 1)

Now we begin to get closer to the truth. Experimentation is still ill defined but is clearly an important part of the mathematical process. It is clearly not new but by implication must be inelegant, lopsided and lax. We, of course, dispute all three of these points and while we do not reply directly to these charges, we hope the reader will be convinced that there need be no compromises made with respect to the quality of the work.

But what is the journal interested in publishing? Their goal seems to be two-fold.

While we value the theorem-proof method of exposition, and while we do not depart from the established view that a result can only become part of mathematical knowledge once it is supported by a logical proof, we consider it anomalous that an important component of the process of mathematical creation is hidden from public discussion. It is to our loss that most of the mathematical community are almost always unaware of how new results have been discovered. ([87] p. 1)

and

The early sharing of insights increases the possibility that they will lead to theorems: an interesting conjecture is often formulated by a researcher who lacks the techniques to formalize a proof, while those who have the techniques at their fingertips have been looking elsewhere.

It appears that through the journal Experimental Mathematics the editors advocate a not undramatic change in writing style. So what does a paper published in that journal look like? A recent example is “Experimental Evaluation of Euler sums” by D. H. Bailey, J. Borwein and R. Girgensohn ([20]). The authors describe how their interest in Euler sums was roused by a surprising discovery:

In April 1993, Enrico Au-Yeung, an undergraduate at the University of Waterloo, brought to the attention of one of us the curious
fact that
\[ \sum_{k=1}^{\infty} \left( 1 + \frac{1}{2} + \cdots + \frac{1}{k} \right)^2 k^{-2} = 4.59987 \cdots \]
\[ \approx \frac{17}{4} \zeta(4) = \frac{17\pi^4}{360} \]

based on a computation to 500,000 terms. This author’s reaction was to compute the value of this constant to a higher level of precision in order to dispel this conjecture. Surprisingly, a computation to 30 and later to 100 decimal digits still affirmed it. (20 p. 17)

This type of serendipitous discovery must go on all the time, but it needs the flash of insight that will place it in a broader context. It is like a gold nugget waiting to be refined—without a context it would remain a curiosity. The authors now proceeded to provide a context by mounting a full-fledged assault on the problem. They systematically applied an integer relation detection algorithm to large classes of sums of the above type, trying to find evaluations of these sums in terms of zeta functions (see Table 7.1 and 7.2 for details). Some of the experimentally discovered evaluations were then proven rigorously, others remain conjectures. While Au-Yeung’s insight may fill us with a sense of amazement, the experimenters’ approach appears quite natural and systematic.
Experimental Approach

1. Employ an advanced scheme to compute high-precision (100+ digit) numerical values for various constants in a class.
2. Conjecture the form of terms involved in possible closed-form evaluations.
3. Employ an integer relation finding algorithm to determine if an Euler sum value is given by a rational linear combination of the conjectured terms.
4. Attempt to find rigorous proofs of experimental results.
5. Attempt to generalize proofs for specific cases to general classes of Euler sums.

Table 7.1. Serendipity and experimentation.
Definitions:

\[ \zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^s} \]

\[ s_h(m, n) = \sum_{k=1}^{\infty} \left( 1 + \frac{1}{2} + \cdots + \frac{1}{k} \right)^m (k + 1)^{-n} \quad m \geq 1, \ n \geq 2 \]

Some experimentally derived conjectures:

\[ s_h(3, 2) = \frac{15}{2} \zeta(5) + \zeta(2) \zeta(3) \]
\[ s_h(3, 3) = -\frac{33}{16} \zeta(6) + 2 \zeta^2(3) \]
\[ s_h(3, 4) = \frac{119}{16} \zeta(7) - \frac{33}{4} \zeta(3) \zeta(4) + 2 \zeta(2) \zeta(5) \]
\[ s_h(3, 6) = \frac{197}{24} \zeta(9) - \frac{33}{7} \zeta(4) \zeta(5) - \frac{37}{8} \zeta(3) \zeta(6) + \zeta^3(3) + 3 \zeta(2) \zeta(7) \]
\[ s_h(4, 2) = \frac{859}{24} \zeta(6) + 3 \zeta^2(3) \]

We are given the raw data with which to work, carefully organized to give us a glimpse into the investigators’ insights on the problem. Note in the first formula for \( s_h(3, 2) \), \( 3 + 2 = 5 \), on the right hand side of the equation we have \( \zeta(5) \) and \( \zeta(3) \zeta(2) \).

Some proven Euler sums:

\[ s_h(2, 2) = \frac{3}{2} \zeta(4) + \frac{1}{2} \zeta^2(2) = \frac{11\pi^4}{360} \]
\[ s_h(2, 4) = \frac{2}{3} \zeta(6) - \frac{1}{3} \zeta(2) \zeta(4) + \frac{1}{3} \zeta^3(2) - \zeta^2(3) = \frac{37\pi^6}{22680} - \zeta^3(3) \]

The proven evaluation for \( s_h(2, 2) \) above implies the truth of Au-Yeung’s discovery.

Table 7.2. Some experimental results.

The editors of Experimental Mathematics are advocating a change in the way mathematics is written, placing more emphasis on the mathematical process. Imre Lakatos in his influential though controversial book *Proofs and Refutations* [138] advocated a similar change from what he called the deductivist style of proof to the heuristic style of proof. In the deductivist style, the definitions are carefully tailored to the proofs. The proofs are frequently elegant and short. But it is difficult to see what process led to the discovery of the theorem and its proof. The heuristic style maintains the
7.2. Experimental Mathematics

mathematical rigor but again the emphasis is more on process. One does not merely give the definition but perhaps includes a comment on why this definition was chosen and not another. This is clearly an important shift if the editors wish to meet their second objective, the sharing of insights.

7.2.2 The Deductivist Style

The major focus of this section is Imre Lakatos’s description of the deductivist style in *Proofs and Refutations*. An extreme example of this style is given in the form of a computer generated proof of $(1 + 1)^n = 2^n$ in Table 7.3.

Euclidean Methodology has developed a certain obligatory style of presentation. I shall refer to this as “deductivist style.” This style starts with a painstakingly stated list of *axioms, lemmas* and/or *definitions*. The axioms and definitions frequently look artificial and mystifyingly complicated. One is never told how these complications arose. The list of axioms and definitions is followed by the carefully worded *theorems*. These are loaded with heavy-going conditions; it seems impossible that anyone should ever have guessed them. The theorem is followed by the *proof*. ([138] p. 142)

When one first learns to sum infinite series one is taught to sum geometric series

$$1 + \rho + \rho^2 + \cdots + \rho^k + \cdots = \frac{1}{1 - \rho}$$

when $|\rho| < 1$. Next one learns to sum telescoping series. For example if $f(i) = \frac{1}{i+1} - \frac{1}{i+2}$, it is not to hard to see that

$$\sum_{i=0}^{n} f(i) = (1 - \frac{1}{2}) + (\frac{1}{2} - \frac{1}{3}) \cdots (\frac{1}{n+1} - \frac{1}{n+2}) = 1 - \frac{1}{n+2}$$

and in particular that

$$\sum_{i=0}^{\infty} f(i) = 1.$$

The Wölf-Zeilberger algorithms employ “creative telescoping” to show that a sum or integral is zero. The algorithms really provide a meta-insight into a broad range of problems involving identities. Unfortunately the proofs produced by the computer, while understandable by most mathematicians are at the same time uninteresting. On the other hand, the existence of WZ proofs for large classes of objects gives us a global insight into these areas.

Table 7.3. Shrinking or encapsulating mathematics.
This is the essence of what we have called formal understanding. We know that the results are true because we have gone through the crucible of the mathematical process and what remains is the essence of truth. But the insight and thought processes that led to the result are hidden.

In deductivist style, all propositions are true and all inferences valid. Mathematics is presented as an ever-increasing set of eternal, immutable truths. (138 p. 142)

Deductivist style hides the struggle, hides the adventure. The whole story vanishes, the successive tentative formulations of the theorem in the course of the proof-procedure are doomed to oblivion while the end result is exalted into sacred infallibility. (138 p. 142)

Perhaps the most extreme examples of the deductivist style come out of the computer generated proofs guaranteed by Wilf and Zeilberger’s algorithmic proof theory. It is important to note here that Wilf and Zeilberger transform the problem of proving identities to the more computer oriented problem of solving a system of linear equations with symbolic coefficients.

These WZ proofs (see Table 7.4) are perhaps the ultimate in the deductivist tradition. At present, knowing the WZ proof of an identity amounts to little more (We will discuss the importance of certificates later.) than knowing that the identity is true. In fact, Doron Zeilberger in 196 has advocated leaving only a QED at the end of the statement, the author’s seal that he has had the computer perform the calculations needed to prove the identity. The advantage of this approach is that the result is completely encapsulated. Just as one would not worry about how the computer multiplied two huge integers together or inverted a matrix, one now has results whose proofs are uninteresting.

7.3 Zeilberger and the Encapsulation of Identity

7.3.1 Putting a Price on Reliability

In the last two sections we talked about the importance of communicating insights within the mathematical community. There we focused on the process of mathematical thought but now we want to talk about communicating insights that have not been made rigorous.

We have already briefly talked about Wilf and Zeilberger’s algorithmic proof theory and its denial of insight. In this section we will discuss the implications of this theory and D. Zeilberger’s philosophy of mathematics
7.3. Zeilberger and the Encapsulation of Identity

Below is a sample WZ proof of \((1 + 1)^n = 2^n\) (this proof is a modified version of the output of Doron Zeilberger’s original Maple program, influenced by the proof in [199]).

Let \(F(n, k) = \binom{n}{k} 2^{-n}\). We have to show that \(l(n) = \sum_k F(n, k) = 1\). To do this we will show that \(l(n+1) - l(n) = 0\) for every \(n \geq 0\) and that \(l(0) = 1\). The second half is trivial since for \(n = 0\), \(F(0, 0)\) is equal to 1 and 0 otherwise. The first half is proved by the WZ algorithm.

We construct

\[
G(n, k) = -\frac{1}{2(n+1)} \binom{n}{k-1} \left( -\frac{k}{2(n-k+1)} F(n, k) \right),
\]

with the motive that

\[
WZ = F(n+1, k) - F(n, k) = G(n, k+1) - G(n, k) \quad \text{(check!).}
\]

Summing WZ with respect to \(k\) gives

\[
\sum_k F(n+1, k) - \sum_k F(n, k) = \sum_k (G(n, k+1) - G(n, k)) = 0
\]

(by telescoping). We have now established that \(l(n+1) - l(n) = 0\) and we are done.

The proof gives little insight into this binomial coefficient identity. However, the algorithms give researchers in other fields direct access to the field of special function identities.

Table 7.4. An uninteresting(?) proof.

as contained in Theorems for a Price: Tomorrow’s Semi-Rigorous Mathematical Culture ([197]).

It is probably unfortunate but perhaps necessary that the two voices most strongly advocating truly experimental math are also at times the most hyperbolic in their language. We will concentrate mostly on the ideas of Doron Zeilberger but G. J. Chaitin should not and will not be ignored.

We will begin with D. Zeilberger’s “Abstract of the future”

We show in a certain precise sense that the Goldbach conjecture is true with probability larger than 0.99999 and that its complete truth could be determined with a budget of 10 billion. ([197], p. 980)

Once people get over the shock of seeing probabilities assigned to truth in mathematics the usual complaint is that the 10 billion is ridiculous.
Computers have been getting better and cheaper for years. What can it mean that “the complete truth could be determined with a budget of 10 billion?” What is clear from the article is that this is an additive measure of the difficulty of completely solving this problem. If we know that the Riemann hypothesis will be proven if we prove lemmas costing 10 billion, 2 billion and 2 trillion dollars respectively, we can tell at a glance not merely what it would “cost” to prove the hypothesis but also where new ideas will be essential in any proof. (This assumes that 2 trillion is a lot of “money.”)

The introduction of “cost” leads immediately to consideration of a trend that has over taken the business world and is now intruding rapidly on academia: a focus on productivity and efficiency.

It is a waste of money to get absolute certainty, unless the conjectured identity in question is known to imply the Riemann Hypothesis (p. 980)

We have taken this quote out of its context (Wilf and Zeilberger’s algorithmic proof theory of identities) but even so we think it is indicative of a small but growing group of mathematicians who are asking us to look at not just the benefits of reliability in mathematics but also the associated costs. See for example A. Jaffe and F. Quinn in [119, 120] and G. Chaitin in [66]. Still, we have not dealt with the central question. Why does D. Zeilberger need to introduce probabilistic “truths?” and how might we from a “formalist” perspective not feel this to be a great sacrifice?

7.3.2 It’s All About Insight

Why is Zeilberger so willing to give up on absolute truths? The most reasonable answer is that he is pursuing deeper truths. In *Identities in Search of Identities*, Zeilberger advocates an examination of identities for the sake of studying identities. Still as Herb Wilf and others have pointed out it is possible to produce an unlimited number of identities. It is the context, the ability to use and manipulate these identities, that make them interesting. Why then might we think that studying identities for their own sake may lead us down the golden path rather than the garden path?

We are now looking for what might be called meta-mathematical structures. We remove the math from its original context and isolate it, trying to detect new structures. When doing this it is impossible to collect only the relevant information that will lead to the new discovery. One collects objects (theorems, statistics, conjectures, etc.) that have a reasonable degree of similarity and familiarity and then attempts to eliminate the irrelevant or the untrue (counter examples). We are preparing for some form of eliminative induction. There is a built in stage, where objects are subject to
7.3. Zeilberger and the Encapsulation of Identity

censorship. In this context, it is not unreasonable to introduce objects where one is not sure of their truth, since all the objects, whether proved or not, will be subject to the same degree of scrutiny. Moreover, if these probably true objects fall into the class of reliable (i.e., they fit the new conjecture) objects, it may be possible to find a legitimate proof in the new context. Recall that the fast WZ algorithms transform the problem of proving an identity to one of solving a system of linear equations with symbolic coefficients.

It is very time consuming to solve a system of linear equations with symbolic coefficients. By plugging in specific values for $n$ and other parameters if present, one gets a system with numerical coefficients, which is much faster to handle. Since it is unlikely that a random system of inhomogeneous linear equations with more equations than unknowns can be solved, the solvability of the system for a number of special values of $n$ and the other parameters is a very good indication that the identity is indeed true. (1977, p. 980)

Suppose we can solve the system above for ten different assignments for $n$ and the other parameters but cannot solve the general system. What do we do if we really need this identity? We are in a peculiar position. We have reduced the problem of proving identities involving sums and integrals of proper-hypergeometric terms to the problem of solving a possibly gigantic system of inhomogeneous linear equations with more equations than unknowns. We have an appropriately strong belief that this system has a solution but do not have the resources to uncover this solution.

What can we do with our result? If we agree with G. J. Chaitin, we may want to introduce it as an “axiom.”

I believe that elementary number theory and the rest of mathematics should be pursued more in the spirit of experimental science, and that you should be willing to adopt new principles. I believe that Euclid’s statement that an axiom is a self-evident truth is a big mistake. The Schrödinger equation certainly isn’t a self-evident truth! And the Riemann Hypothesis isn’t self-evident either, but it’s very useful. A physicist would say that there is ample experimental evidence for the Riemann Hypothesis and would go ahead and take it as a working assumption. (66, p. 24)

In this case, we have ample experimental evidence for the truth of our identity and we may want to take it as something more than just a working assumption. We may want to introduce it formally into our mathematical system.

There is no evidence that Euclid ever made such a statement. However, the statement does have an undeniable emotional appeal.
7.4 Experiment and “Theory”

We have now examined two views of experimental mathematics but we appear to be no closer to a definition than when we began. However, we are now ready to begin in full our exploration of experiment. In *Advice to a Young Scientist*, P. B. Medawar defines four different kinds of experiment: the Kantian, Baconian, Aristotelian, and the Galilean. Mathematics has always participated deeply in the first three categories but has somehow managed to avoid employing the Galilean model. In developing our notion of experimental mathematics we will try to adhere to this Galilean mode as much as possible.

We will begin with the Kantian experiments. Medawar gives as his example:

> generating “the classical non-Euclidean geometries (hyperbolic, elliptic) by replacing Euclid’s axiom of parallels (or something equivalent to it) with alternative forms.” ([153] pp. 73–74)

It seems clear that mathematicians will have difficulty escaping from the Kantian fold. Even a Platonist must concede that mathematics is only accessible through the human mind and thus at a basic level all mathematics might be considered a Kantian experiment. We can debate whether Euclidean geometry is but an idealization of the geometry of nature (where a point has no length or breadth and a line has length but no breadth?) or nature an imperfect reflection of “pure” geometrical objects, but in either case the objects of interest lie within the minds eye.

Similarly, we cannot escape the Baconian experiment. In Medawar’s words this

> is a contrived as opposed to a natural happening, it “is the consequence of ‘trying things out’ or even of merely messing about.” ([153] p. 69)

Most of the research described as experimental is Baconian in nature and in fact one can argue that all of mathematics proceeds out of Baconian experiments. One tries out a transformation here, an identity there, examines what happens when one weakens this condition or strengthens that one. Even the application of probabilistic arguments in number theory can be seen as a Baconian experiment. The experiments may be well thought out and very likely to succeed but the ultimate criteria of inclusion of the result in the literature is success or failure. If the “messing about” works (e.g., the theorem is proved, the counterexample found) the material is kept; otherwise, it is relegated to the scrap heap.

The Aristotelian experiments are described as demonstrations:
apply electrodes to a frog’s sciatic nerve, and lo, the leg kicks; always precede the presentation of the dog’s dinner with the ringing of a bell, and lo, the bell alone will soon make the dog dribble. ([153] p. 71)

The results are tailored to demonstrate the theorems, as opposed to the experiments being used to devise and revise the theorems. This may seem to have little to do with mathematics but it has everything to do with pedagogy. The Aristotelian experiment is equivalent to the concrete examples we employ to help explain our definitions, theorems, or the problems assigned to students so they can see how their newly learned tools will work.

The last and most important is the Galilean experiment:

(the) Galilean Experiment is a critical experiment—one that discriminates between possibilities and, in doing so, either gives us confidence in the view we are taking or makes us think it in need of correction. ([153])

Ideally one devises an experiment to distinguish between two or more competing hypotheses. In subjects like medicine the questions are in principal more clear cut (the Will Roger’s phenomenon or Simpson’s paradox complicates matters). Does this medicine work (longevity, quality of life, cost effectiveness, etc.)? Is this treatment better than that one? Unfortunately, these questions are extremely difficult to answer and the model Medawar presents here does not correspond with the current view of experimentation. Since the spectacular “failure” (i.e., it worked beautifully but ultimately was supplanted see [139]) of Newtonian physics it has been widely held that no amount of experimental evidence can prove or disprove a theorem about the world around us and it is widely known that in the real world the models one tests are not true. Medawar acknowledges the difficulty of proving a result but has more confidence than modern philosophers in disproving hypotheses. If experiment cannot distinguish between hypotheses or prove theorems, what can it do? What advantages does it have? Is it necessary?

7.5 “Theoretical” Experimentation

While there is an ongoing crisis in mathematics, it is not as severe as the crisis in physics. The untestability of parts of theoretical physics (e.g., string

\textsuperscript{5}Simpson’s paradox notes that two data sets can separately support one conclusion while the union of the data supports the opposite conclusion. Will Roger’s phenomenon notes that in a medical study it is possible to transfer a patient from one group to another and improve the statistics of both groups.
theory) has led to a greater reliance on mathematics for “experimental verification.” This may be in part what led Arthur Jaffe and Frank Quinn to advocate what they have named “Theoretical Mathematics” (note that many mathematicians think they have been doing theoretical mathematics for years) but which we like to think of as “theoretical experimentation.” There are certainly some differences between our ideas and theirs but we believe they are more of emphasis than substance.

Unlike our initial experiment where we are working with and manipulating floating point numbers, “theoretical experimentation” would deal directly with theorems, conjectures, the consequences of introducing new axioms. ... Note that by placing it in the realm of experimentation, we shift the focus from the more general realm of mathematics, which concerns itself with the transmission of both truth and insight, to the realm of experimentation, which primarily deals with the establishment of and transmission of insight. Although it was originally conceived outside the experimental framework, the central problems Jaffe and Quinn need to deal with are the same. They must attempt to preserve the rigorous core of mathematics, while contributing to an increased understanding of mathematics both formally and intuitively.

As described in Arthur Jaffe and Frank Quinn’s “Theoretical Mathematics: Toward a Cultural Synthesis of Mathematics and Theoretical Physics” it appears to be mainly a call for a loosening of the bonds of rigor. They suggest the creation of a branch of theoretical (experimental) mathematics akin to theoretical physics, where one produces speculative and intuitive works that will later be made reliable through proof. They are concerned about the slow pace of mathematical developments when all the work must be rigorously developed prior to publication. They argue convincingly that a haphazard introduction of conjectorial mathematics will almost undoubtedly result in chaos.

Their solution to the problems involved in the creation of theoretical (experimental) mathematics comes in two parts. They suggest that

theoretical work should be explicitly acknowledged as theoretical and incomplete; in particular, a major share of credit for the final result must be reserved for the rigorous work that validates it. ([119] p.10)

This is meant to ensure that there are incentives for following up and proving the conjectured results.

To guarantee that work in this theoretical mode does not affect the reliability of mathematics in general, they propose a linguistic shift.

Within a paper, standard nomenclature should prevail: in theoretical material, a word like “conjecture” should replace “theorem”; a
word like “predict” should replace “show” or “construct”; and ex-
pressions such as “motivation” or “supporting argument” should re-
place “proof.” Ideally the title and abstract should contain a word
like “theoretical”, “speculative”, or “conjectural”. (119 p.10)

Still, none of the newly suggested nomenclature would be entirely out of
place in a current research paper. Speculative comments have always had
and will always have a place in mathematics.

This is clearly an exploratory form of mathematics. But is it truly
experimental in any but the Baconian sense? The answer will of course lie
in its application. If we accept the description at face value, all we have is a
lessening of rigor, covered by the introduction of a new linguistic structure.
More “mathematics” will be produced but it is not clear that this math
will be worth more, or even as much as, the math that would have been
done without it.

It is not enough to say that mathematical rigor is strangling mathe-
matical productivity. One needs to argue that by relaxing the strictures
temporarily one can achieve more. If we view theoretical (experimental)
mathematics as a form of Galilean experimentation then in its idealized
form “theoretical” (experimental) mathematics should choose between di-
rections (hypotheses) in mathematics. Like any experimental result the
answers will not be conclusive, but they will need to be strong enough to
be worth acting on.

Writing in this mode, a good theoretical paper should do more than just
sketch arguments and motivations. Such a paper should be an extension
of the survey paper, defining not what has been done in the field but what
the author feels can be done, should be done and might be done, as well
as documenting what is known, where the bottlenecks are, etc. In general,
we sympathize with the desire to create a “theoretical” mathematics but
without a formal structure and methodology it seems unlikely to have the
focus required to succeed as a separate field.

One final comment seems in order here. “Theoretical” mathematics, as
practiced today, seems a vital and growing institution. Mathematicians
now routinely include conjectures and insights with their work (a trend
that seems to be growing). This has expanded in haphazard fashion to
include algorithms, suggested algorithms and even pseudo algorithms. We
would distinguish our vision of “experimental” mathematics from “theoretical”
mathematics by an emphasis on the constructive/algorithmic side of
mathematics. There are well established ways of dealing with conjectures
but the rules for algorithms are less well defined. Unlike most conjectures,
algorithms if sufficiently efficacious soon find their way into general use.

While there has been much discussion of setting up standardized data
bases to run algorithms on, this has proceeded even more haphazardly.
Addressing these issues of reliability would be part of the purview of experimental mathematics. Not only would one get a critical evaluation of these algorithms but by reducing the problems to their algorithmic core, one may facilitate the sharing of insights both within and between disciplines. At its most extreme, a researcher from one discipline may not need to understand anything more than the outline of the algorithm to make important connections between fields.

7.6 A Mathematical Experiment

7.6.1 Experimentation

We now turn to a more concrete example of a mathematical experiment. Our meta-goal in devising this experiment was to investigate the similarities and differences between experiments in mathematics and in the natural sciences, particularly in physics. We therefore resolved to examine a conjecture which could be approached by collecting and investigating a huge amount of data: the conjecture that every non-rational algebraic number is normal in every base (see Table 7.5). It is important to understand that we did not aim to prove or disprove this conjecture; our aim was to find evidence pointing in one or the other direction. We were hoping to gain insight into the nature of the problem from an experimental perspective.

The actual experiment consisted of computing to 10,000 decimal digits the square roots and cube roots of the positive integers smaller than 1000 and then subjecting these data to certain statistical tests (again, see Table 7.5). Under the hypothesis that the digits of these numbers are uniformly distributed (a much weaker hypothesis than normality of these numbers), we expected the probability values of the statistics to be distributed uniformly between 0 and 1. Our first run showed fairly conclusively that the digits were distributed uniformly. In fact, the Anderson-Darling test, which we used to measure how uniformly distributed our probabilities were suggested that the probabilities might have been “too uniform” to be random. We therefore ran the same tests again, only this time for the first 20,000 decimal digits, hoping to detect some non-randomness in the data. The data were not as interesting on the second run.

7.6.2 Verification

It is even more important in mathematics than in the physical sciences that the data under investigation are completely reliable. At first glance it may seem that the increasing reliance of mathematicians on programs such as Maple and Mathematica, has decreased the need for verification.
Definition. A real number is normal to the base 10 if every block of digits of length $k$ occurs with frequency $1/10^k$.

Example: the Champernowne number

$0.01234567891011121314\ldots 99100101\ldots$

is known to be normal base 10.

Except for artificially created examples no numbers have been proven normal in any particular base. If we allow artificial numbers there are no explicit numbers known to be normal in every base.

Questions:

- Are all non-rational algebraic numbers normal base 10?
- Do all non-rational algebraic numbers have uniformly distributed digits?

G. J. Chaitin in *Randomness and Complexity in Pure Mathematics*, has a number he calls $\Omega = \sum_p \text{halts}_2 2^{-|p|}$, the halting probability, which he notes is “sort of a mathematical pun”, but is normal to all bases. He does this by identifying integers with binary strings representing Turing machines and summing over the programs that stopped (non-trivially, see [66] p.12).

Table 7.5. Background on normality.

Computers very rarely make arbitrary mistakes in arithmetic and algebra. But all the systems have known and unknown bugs in their programming. It is therefore imperative that we check our results. So what efforts did we take to verify our findings?

First of all, we had to make sure that the roots we computed were accurate to at least 10,000 (resp. 20,000) digits. We computed these roots using Maple as well as Mathematica, having them compute the roots to an accuracy of 10,010 digits. We then did two checks on the computed approximation $s_n$ to $\sqrt{n}$. First, we tested that $\sqrt{n} \in [s_n - 10^{-10005}, s_n + 10^{-10005}]$ by checking that $(s_n - 10^{-10005})^2 < n < (s_n + 10^{-10005})^2$. Second, we tested that the 10,000th through 10,005th digits were not all zeroes or nines. This ensures that we actually computed the first 10,000 digits of the decimal expansion of $\sqrt{n}$. (We note that Maple initially did not give us an accuracy of 10,000 digits for all of the cube roots, so that we had to increase the precision.)

We then had to make sure that we computed the statistics and probability values accurately—or at least to a reasonable precision, since we used asymptotic formulas anyway. We did this by implementing them both in Maple and in Mathematica and comparing the results. We detected no significant discrepancy.

We claim that these measures reasonably ensure the reliability of our experimental results.
We looked at the first 10,000 digits after the decimal point of the $\sqrt{n}$ where $n < 1000$ is not a perfect square and of $\sqrt[3]{n}$ where $n < 1000$ is not a perfect cube.

Tests used:
- $\chi^2$—to check that each digit occurs 1/10 of the time (discrete uniform distribution base 10).
- Discrete Cramér-von Mises—to check that all groups of 4 consecutive digits occurs 1/10,000 of the time (discrete uniform distribution base 10,000).
- Anderson-Stephens—to check that the power spectrum of the sequence matches that of white noise (periodicity).
- Anderson-Darling—continuous uniform distribution.

Important point: In order for us to claim we have generated any evidence at all either for or against we have made two fairly strong assumptions.
- The first 10,000 digits are representative of the remaining digits.
- These digits behave as far as our statistical tests go like independent random variables.

In fact, for the first and second 10,000 digits our final conclusions are identical. The second assumption is problematic. Since we have beautiful algorithms to calculate these numbers, by most reasonable definitions of independent and random, these digits are neither.

Table 7.6. Data and statistics.

7.6.3 Interpretation

Our experimental results support the conjecture that every non-rational algebraic number is normal; more precisely, we have found no evidence against this conjecture. In this section we will describe how we looked at and interpreted the experimental data to arrive at this conclusion. We include only a few examples of how we looked at the data here. In fact, we have only looked at certain aspects of normality and randomness in decimal expansions. Thus our results may be interpreted more narrowly to support the hypothesis that algebraic numbers are normal base 10. A full description will be found in [51].

Our main goal here is to give a quick visual summary that is at once convincing and data rich. These employ some of the most basic tools of visual data analysis and should probably form part of the basic vocabulary of an experimental mathematician. Note that traditionally one would run a test such as the Anderson-Darling test (which we have done) for the continuous uniform distribution and associate a particular
probability with each of our sets of probability, but unless the probability values are extremely high or low it is difficult to interpret these statistics.

Experimentally, we want to test graphically the hypothesis of normality and randomness (or non-periodicity) for our numbers. Because the statistics themselves do not fall into the nicest of distributions, we have chosen to plot only the associated probabilities. We include two different types of graphs here. A quantile-quantile plot is used to examine the distribution of our data and scatter plots are used to check for correlations between statistics.

The first is a quantile-quantile plot of the chi square base 10 probability values versus a discrete uniform distribution. For this graph we have placed the probabilities obtained from our square roots and plotted them against a perfectly uniform distribution. Finding nothing here is equivalent to seeing that the graph is a straight line with slope one. This is a crude but effective way of seeing the data. The disadvantage is that the data are really plotted along a one dimensional curve and as such it may be impossible to see more subtle patterns.

The other graphs are examples of scatter plots. The first scatter plot shows that nothing interesting is occurring. We are again looking at probability values this time derived from the discrete Cramer-von Mises (CVM) test base 10,000. For each cube root we have plotted the point \((f_i, s_i)\), where \(f_i\) is the CVM base 10,000 probability associated with the first 2500 digits of the cube root of \(i\) and \(s_i\) is the probability associated with the next 2500 digits. A look at the graph reveals that we have now plotted our data on a two dimensional surface and there is a lot more "structure" to be seen. Still, it is not hard to convince oneself that there is little or no relationship between the probabilities of the first 2500 digits and the second 2500 digits.

The last graph is similar to the second. Here we have plotted the probabilities associated with the Anderson-Stephens statistic of the first 10,000 digits versus the first 20,000 digits. We expect to find a correlation between these tests since there is a 10,000 digit overlap. In fact, although the effect is slight, one can definitely see the thinning out of points from the upper left hand corner and lower right hand corner.

7.7 Conclusion

All the versions of experimental mathematics that we have dealt with so far have two characteristics: their main interest is in expanding our mathemat-
Figure 7.1. Graphical statistics of our experiments.
7.7. Conclusion

Mathematical knowledge as rapidly as possible and none of them stray too far from the mainstream. In many cases this urgency leads to a temporary relaxation of rigor, a relaxation that is well documented and hopefully can be cleaned up afterwards. In other cases it may be intrinsic to the mathematics they wish to explore. When a field has been as wildly successful as mathematics has been in the past few centuries there is a reluctance to change. We have hoped to convince some of the readers that these changes are revolutionary only in the same sense that the earth revolves around the sun.

We conclude with a definition of experimental mathematics.

**Experimental Mathematics** is that branch of mathematics that concerns itself ultimately with the codification and transmission of insights within the mathematical community through the use of experimental (in either the Galilean, Baconian, Aristotelian or Kantian sense) exploration of conjectures and more informal beliefs and a careful analysis of the data acquired in this pursuit.

Results discovered experimentally will, in general, lack some of the rigor associated with mathematics but will provide general insights into mathematical problems to guide further exploration, either experimental or traditional. We have restricted our definition of experimental mathematics to methodological pursuits that in some way mimic Medawar’s views of Galilean experimentation. However, our emphasis on insight also calls for the judicious use of examples (Aristotelian experimentation).

If the mathematical community as a whole was less splintered, we would probably remove the word “codification” from the definition. That is to say that a great deal of time will need to be spent on developing a language for the expression of experimental results. Since there are real communications problems between fields and since the questions to be explored will be difficult, it seems imperative that experimental investigators make every effort to organize their insights and present their data in a manner that will be as widely accessible as possible.

With respect to reliability and rigor, the main tools here are already in place. We need to stress systematization of our exploration. As in our experimental project on normality, it is important to clearly define what has been looked at, how things have been examined, and what confidence the reader should have in the data. Although mathematicians may not like to admit it, ease of use will have to be a primary consideration if experimental results are to be of widespread use. As such, visualization and hypertextual presentations of material will become increasingly important.

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6It is clear that mechanisms are developing for transmitting insights within fields, even if this is only through personal communications.
in the future. We began by stealing some of the basic tools of scientific analysis and laying claim to them. As the needs of the community become more apparent one would expect these tools and others to evolve into a form better suited to the particular needs of the mathematical community. Someday, who knows, first year graduate students may be signing up for Experimental Methods in Mathematics I.
A Color Supplement
Color Plate I. Pascal triangles modulo two? (See Figure 2.1).

Color Plate II. Root two is irrational (See Figure 2.11).
Color Plate III. Projection of 4-D polyhedron (See Figure 2.16).

Color Plate IV. Ferguson’s “Eight-Fold Way” and “Figure-Eight Knot Complement” (See Figures 2.4 and 2.5).
Color Plate V. Ferguson’s “Invisible Handshake” (See Figure 2.17).

Color Plate VI. The “Firmament” by John Robinson (See Figure 2.15).
Color Plate VII. Coxeter’s own kaleidoscope model (See Figure 2.14).
Color Plate VIII. A random walk based on one million digits of $\pi$ (See Figure 4.1).
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