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Preface

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

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

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

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

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

Our views have been expressed well by Epstein and Levy in a 1995 article on experiment and proof [135].

> 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* [234]. 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: [157] and [202]. In both cases, however, the focus and scope centers on the teaching of students and thus is quite different from ours.

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

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Experimental Mathematics Web Site

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

Jonathan M. Borwein
David H. Bailey
August 2003

Preface to the CD-ROM Edition of 2006

Even in the short time since the First edition of our two books, *Mathematics by Experiment: Plausible Reasoning in the 21st Century* and *Experimentation in Mathematics: Computational Paths to Discovery*, there has been a noticeable upsurge in interest in using computers to do real mathematics. One measure of this interest is the large number of email messages that we have received from researchers, previously unknown to us, who are engaged in similar work, and who have obtained interesting new results. Another indication is the corresponding increase in the number of papers being written and published in this area.

In our own research, we have noted how often we ourselves refer to the PDF files of our books, which we use to do searches to and a passage or a discussion of interest. After some discussions with our publisher, Klaus Peters, we concluded that the usability of these books would be greatly enhanced if these PDF files could be made available, while at the same time updating these PDF files with some corrections that have been noted by our colleagues since the books were first published. To maintain fidelity with the published version, we have typically not updated either textual material or the bibliography. But we also decided to do more than just release the revised editions of these books on a CD-ROM. We have also devised, with the able help of several research assistants, several "smart" enhancements. We also wish to emphasize our website, which we have established expressly for the purpose of supporting these books: `http://www.experimentalmath.info`. Note that this is different than the one we included in the first editions of the books, namely http://www.expmath.info, although this latter URL will continue to be supported in- definitely. Moreover, URLs have a habit of changing. For example, many CECM links have recently migrated to http://oldweb.cecm.sfu.ca (as the site will tell you). A few are no longer accessible and when we believe this to be the case we have left them for archival purposes but have changed their color.

This website also contains updated errata for each volume, available at:
`http://www.experimentalmath.info/books/v1-errata.pdf`
`http://www.experimentalmath.info/books/v2-errata.pdf`
`http://www.experimentalmath.info/books/cd-errata.pdf`

Since the books were originally published, a number of interesting reviews have been published, including the following:

- Review of *Mathematics by Experiment* in *Math Reviews* (Nov. 2004):
  `http://www.experimentalmath.info/books/mr-mbye.pdf`

- Review of *Experimentation in Mathematics* in *Math Reviews* (May 2005):
  `http://www.experimentalmath.info/books/mr-einm.pdf`

- MAA online book review:
  `http://www.maa.org/reviews/experimentalmath.html`

- *American Scientist* review (Mar.–Apr. 2005 issue):
  `http://www.americanscientist.org/template/BookReviewTypeDetail/assetid/40747`

- Review in *Notices of the American Mathematical Society* (Sept. 2005 issue):
  `http://www.experimentalmath.info/books/rev-shallit.pdf`

Many of these include extra references and additional material. In addition to those we thanked in the Preface to the books, we would like to thanks Peter Ye (Dalhousie), Brian Gibson (AK Peters) and Charlotte Henderson (AK Peters) for their careful attention to many details. As before, we would appreciate any comments. Our emails can be found at `http://www.experimentalmath.info`.

Jonathan M. Borwein   David H. Bailey
Roland Girgensohn   Mason Macklem
January 2006

Preface to the Expanded Second Edition of 2008

In this edition, in addition to correcting various minor infelicities and updating references, we have replaced the original Chapter 7 (which was a reprint of a philosophical article [76]) by roughly 100 pages of new material. We wish to thank Peter Borwein, David Bradley, David Broadhurst, Marc Chamberland, O-Yeat Chan, John Cosgrave, Richard Crandall, Karl Dilcher, Frank Garvan, John Holte, Manuel Kauers, Dante Manna, Veronica Pillwein, Mark Pinsky, Andrew Shouldice, Fernando Villegas, and Stan Wagon, among those who have provided interesting material for this supplement. We have also included the expanded symbol index that was constructed for the 2006 CD-ROM joint edition. As before, our thanks go to our friends and editors at AK Peters for their support and care of our work.

Jonathan M. Borwein
David H. Bailey
May 2008

1 | What is Experimental Mathematics?

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

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

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

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

1.1 Background

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

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

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

In the late 1980s, recognizing that its members were lagging behind in embracing computer technology, the American Mathematical Society began a regular "Computers and Mathematics" section in the monthly newsletter, *Notices of the American Mathematical Society*, edited at first by Jon Barwise and subsequently by Keith Devlin. This continued until the mid-1990s and helped to convince the mathematical community that the computer can be a useful research tool. In 1992, a new journal, *Experimental Mathematics*, was launched, founded on the belief "that theory and experiment feed on each other, and that the mathematical community stands to benefit from a more complete exposure to the experimental process." It encouraged the submission of algorithms, results of experiments, and descriptions of computer programs, in addition to formal proofs of new results [134].

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

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

1. Gaining insight and intuition.

2. Discovering new patterns and relationships.

3. Using graphical displays to suggest underlying mathematical principles.

4. Testing and especially falsifying conjectures.

5. Exploring a possible result to see if it is worth formal proof.

6. Suggesting approaches for formal proof.

7. Replacing lengthy hand derivations with computer-based derivations.

8. Confirming analytically derived results.

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

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

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

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

1.2 Complexity Considerations

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

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

> term this rate can be expected to continue, if not to increase. Over
> the longer term, the rate of increase is a bit more uncertain, although
> there is no reason to believe it will not remain nearly constant for at
> least 10 years. [218]

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 [199]. This involved a search for a configuration of $n^2 + n + 1$ points and equally many lines. Lam's computer program required thousands of hours of run time on a Cray computer system. Lam estimates that the next case ($n = 18$) susceptible to his methods would take millions of years on any conceivable architecture.

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

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

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

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

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

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

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

Even with a huge effort, current algorithms get stuck at about 150 digits. Details can be found at `http://www.rsasecurity.com/rsalabs/node.asp?id=2094` where the current factoring challenges are listed. One possible solution to the factorization problem may come through quantum computing, using an algorithm found by Peter Shor in 1994 [257]. However, it is still not clear whether quantum phenomenon can be harnessed on the scale required for this algorithm to be practical.

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

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

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

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

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

The problem can be formulated as follows. Suppose $\mathcal{A}_n$ consists of all sequences $(a_0 = 1, a_1, \cdots, a_n)$ 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 $\mathcal{A}_n$ for each fixed n. This is discussed at length in [82].

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

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

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

1.3 Proof versus Truth

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

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

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

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

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

In the case of computations of digits of π, it has been customary for many years to verify a result either by repeating the computation using a different algorithm, or by repeating with a slightly different index position. For example, if one computes hexadecimal digits of π beginning at position one trillion (we shall see how this can be done in Chapter 3), then this can be checked by repeating the computation at hexadecimal position one trillion minus one. It is easy to verify (see Algorithm 3.0 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 (6.022×10^{23}). Percival's actual computation of the quadrillionth binary digit (i.e., the 250 trillionth hexadecimal digit) of π was verified by a similar scheme, which for brevity we have simplified here.

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

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

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

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

Richard Dedekind's marvelous book, *Two Essays on Number Theory* [128], originally published in 1887, provides a striking example of how the nature of what is a satisfactory proof changes over time. In this work, Dedekind introduces Dedekind cuts and a modern presentation of the construction of the reals (see Item 2 at the end of this chapter). In the second essay, "The Nature and Meaning of Numbers," an equally striking discussion of finite and infinite sets takes place. Therein, one is presented with Theorem 66:

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

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

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

Some other examples of this sort are given by Judith Grabiner, who for instance compares Abel's comments on the lack of rigor in 18th-century arguments with the standards of Cauchy's 19th-century *Cours d'analyse* [150].

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* [159], 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 [233])

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

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

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

> If I can give an abstract proof of something, I'm reasonably happy. But if I can get a concrete, computational proof and actually produce numbers I'm much happier. I'm rather an addict of doing things on computer, because that gives you an explicit criterion of what's going on. I have a visual way of thinking, and I'm happy if I can see a picture of what I'm working with. [240, 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. [121, 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. [231, 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. [194, 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 Ptolemye . . . 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. [137, 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 [284])

1.5 Gauss, the Experimental Mathematician

Carl Friedrich Gauss once confessed

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

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

Here is another example of Gauss's prowess at "mental experimental mathematics." One day in 1799, while examining tables of integrals provided originally by James Stirling, he noticed that the reciprocal of the integral

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

agreed numerically with the limit of the rapidly convergent arithmetic-geometric mean iteration: $a_0 = 1$, $b_0 = \sqrt{2}$;

$$a_{n+1} = \frac{a_n + b_n}{2}, \qquad b_{n+1} = \sqrt{a_n b_n}. \tag{1.1}$$

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 [74, pg. 5] and below) "[the result] will surely open up a whole new field of analysis." He was right. It led to the entire vista of 19th century elliptic and modular function theory.

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

In Figure 1.2, an excited Gauss writes:

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

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

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

Figure 1.1. Gauss on the lemniscate.

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 [241]. As the following two quotes from De Morgan show, neither a pride in numerical skill nor a desire for better geometric tools is new. De Morgan like many others saw profound differences between two and three dimensions:

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

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

Elsewhere, de Morgan celebrates:

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

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

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

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

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

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

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

   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:

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

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 [226].

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" [207]. Discrete geometry (now much in fashion as "computational geometry" and another example of very useful pure mathematics) was clearly more appealing to Sylvester. For Sylvester's theorem (posed but not solved by Sylvester), one can imagine various Java applets but scattering a fair number of points on a sheet of white paper and using a ruler seems more than ample to get a sense of the truth of the result.

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

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

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

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

Dirac conjectured that every sufficiently large set of n noncollinear points contains at least $n/2$ proper (or elementary) lines through exactly two points.
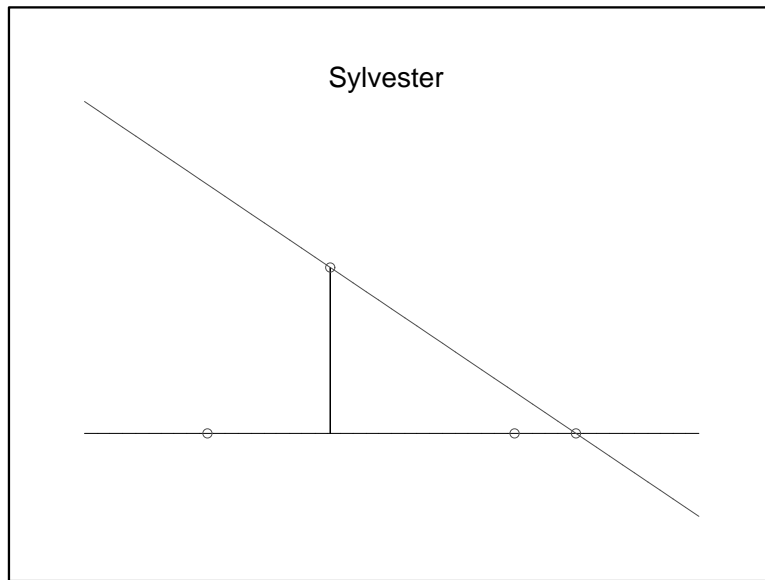
Figure 1.3. Kelly's 1948 "Proof from the Book."

By contrast,

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

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

Sylvester had a most colorful and somewhat difficult life which included
a seminal role in the founding of Johns Hopkins University, and ended as
the first Jewish Chair in Oxford. Educated in Cambridge, he could not
graduate until 1871, when theological tests were finally abolished. This is
engagingly described in *Oxford Figures* [137].

Along this line, readers may be interested in Figures 1.4 and 1.5, which
are taken from Part VII of a 19th century experimental geometry book by
the French educator Paul Bert. The intention was to make school geometry
more intuitive and empirical, quite far from Euclid's *Elements*.
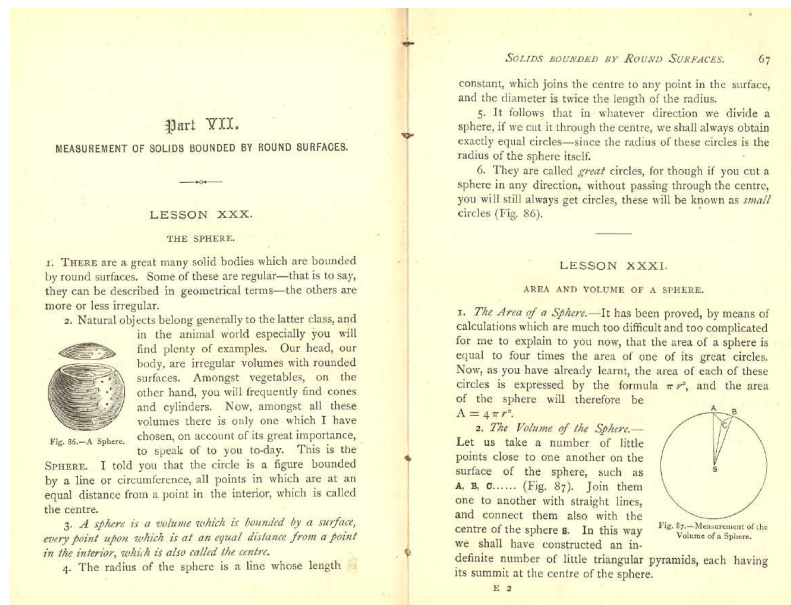
Figure 1.4. Paul Bert's 1886 experimental geometry text, pages 66–67.
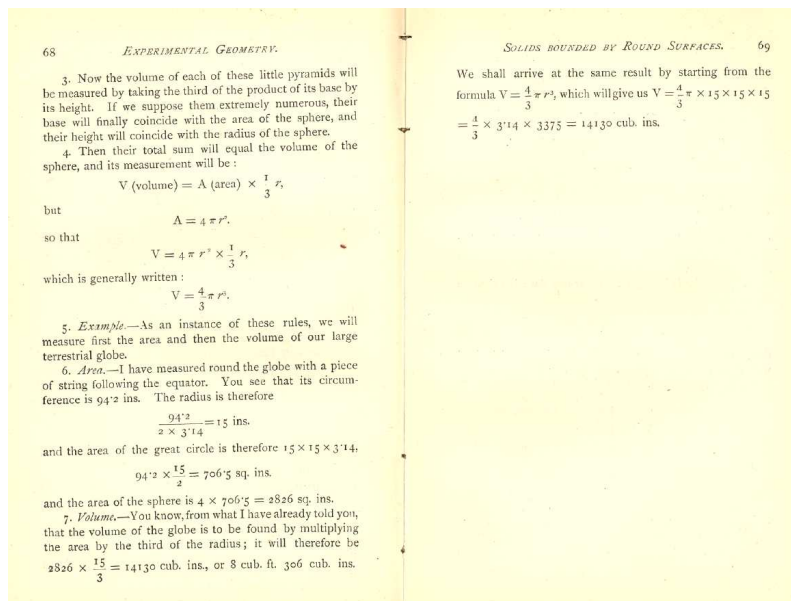
Figure 1.5. Paul Bert's text, pages 68–69.

Figure 1.6. Polya's illustration of the change solution.

1.6.1   On Picture-Writing

George Polya, in an engaging eponymous *American Mathematical Monthly* article, provides three compelling examples of converting pictorial represen- tations of problems into generating function solutions [232]:

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

   This leads to the (US currency) generating function

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

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

   ```
   Series[1/((1-x)*(1-x^5)*(1-x^10)*(1-x^25)*(1-x^50)), {x, 0, 100}]
   ```

   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 $D_3 = 1, D_4 = 2, D_5 = 5, D_6 = 14, D_7 = 42, \dots$

   $$D(x) = \sum_{k=1}^{\infty} D_k x^k$$

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 $\binom{2n}{n}/(n+1)$.

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:

   $$T(x) = \sum_{k=1}^{\infty} T_k x^k = x \prod_{k=1}^{\infty} (1 - x^k)^{-T_k}, \qquad (1.4)$$

   where remarkably the product and the sum share their coefficients. This produces a recursion for T_n in terms of $T_1, T_2, \cdots, T_{n-1}$, which starts: $T_1 = 1, T_2 = 1, T_3 = 2, T_4 = 4, T_5 = 9, T_6 = 20, \cdots$ 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 ℓ^2. What is $||A||$?

4. What is the global minimum of the function $\exp(\sin(50x)) + \sin(60e^y) + \sin(70 \sin x) + \sin(\sin(80y)) - \sin(10(x + y)) + (x^2 + y^2)/4$?

5. Let $f(z) = 1/\Gamma(z)$, where $\Gamma(z)$ is the gamma function, and let $p(z)$ be the cubic polynomial that best approximates $f(z)$ on the unit disk in the supremum norm $|| \cdot ||_\infty$. What is $||f - p||_\infty$?

6. A flea starts at $(0, 0)$ on the infinite 2-D integer lattice and executes a biased random walk: At each step it hops north or south with probability $1/4$, east with probability $1/4 + \epsilon$, and west with probability $1/4 - \epsilon$. The probability that the flea returns to $(0, 0)$ sometime during its wanderings is $1/2$. What is ϵ?

7. Let A be the 20000×20000 matrix whose entries are zero everywhere except for the primes $2, 3, 5, 7, \cdots, 224737$ 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 $I(\alpha) = \int_0^2 [2 + \sin(10\alpha)]x^\alpha \sin(\alpha/(2 - x))\, dx$ depends on the parameter α. What is the value $\alpha \in [0, 5]$ at which $I(\alpha)$ achieves its maximum?

10. A particle at the center of a 10×1 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 [63]. 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, 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 and discussion of techniques for solution are given in [32].

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

$$\sum_{(m,n,p)\neq 0} \frac{(-1)^{m+n+p}}{\sqrt{m^2 + n^2 + p^2}}, \qquad (1.5)$$

   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

$$\sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \cdots + (-1)^{k+1}\frac{1}{k}\right)^2 (k+1)^{-3}.$$

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 $\mathrm{Li}_5(1/2)$, where $\mathrm{Li}_n(x) = \sum_{k>0} x^n/n^k$ 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 π and $\log 2$ are each 1, the degree of $\zeta(3)$ is 3, the degree of $\mathrm{Li}_5(1/2)$ is 5, and the degree of α^n is n times the degree of α.

4. Evaluate

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

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

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

$$R_\eta(a, b) = \cfrac{a}{\eta + \cfrac{b^2}{\eta + \cfrac{4a^2}{\eta + \cfrac{9b^2}{\eta + \ddots}}}}.$$

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

$$\frac{4}{5} \int_0^1 \int_0^1 \int_0^1 \int_0^1 \sqrt{x^2 + y^2 + (z - w)^2}\, dw\, dx\, dy\, dz$$

$$+ \quad \frac{1}{5} \int_0^1 \int_0^1 \int_0^1 \int_0^1 \sqrt{1 + (y - u)^2 + (z - w)^2}\, du\, dw\, dy\, dz.$$

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.

Hint: It is *not* what it first appears to be.

9. Calculate

$$\sum_{i>j>k>l>0} \frac{1}{i^3 j k^3 l}.$$

Extra credit: Express this constant as a single-term expression involving a well-known mathematical constant.

10. Evaluate

$$W_1 \quad = \quad \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{1}{3 - \cos(x) - \cos(y) - \cos(z)}\, dx\, dy\, dz.$$

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 `http://www.experimentalmath.info`.

Institutional Sites

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

2. The American Mathematical Society's Mathematics of Computation journal:
   `http://www.ams.org/mcom`

3. The Association for Computing Machinery's Journal of Experimental Algorithms:
   `http://www.jea.acm.org`

4. Canadian Mathematical Society's KaBoL site:
   `http://camel.math.ca/Kabol`

5. Clay Mathematics Institute:
   `http://www.claymath.org`

6. Experimental Mathematics Journal:
   `http://www.expmath.org`

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

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

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

10. MathSciNet:
    `http://e-math.ams.org/mathscinet`

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

Commercial Sites

1. Apple Computer's Advanced Computation Group research site:
   `http://developer.apple.com/hardware/ve/acgresearch.html`

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`

6. Mathworks (Matlab):
   `http://www.mathworks.com`

7. MathPro Press (online index of math problems and mathematics problem books):
   `http://www.mathpropress.com`

8. The Weisstein-Wolfram Mathworld site:
   `http://mathworld.wolfram.com`

9. The Weisstein-Wolfram Experimental Mathematics site:
   `http://mathworld.wolfram.com/ExperimentalMathematics.html`

10. Wolfram Research, Inc. (*Mathematica*):
    `http://www.wolfram.com`

Noncommercial Software and Tools

1. The 3D-XplorMath Consortium's math visualization tool:
   `http://rsp.math.brandeis.edu/3D-XplorMath/TopLevel/gallery.html`

2. Alf-Christian Achilles' computer science bibliography:
   `http://liinwww.ira.uka.de/bibliography`

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

4. The ArXiv mathematics article database:
   `http://www.arxiv.org`

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

6. The CECM Euler-zeta computation tool:
   `http://oldweb.cecm.sfu.ca/projects/ezface+`

7. The CECM integer relation tool:
   `http://oldweb.cecm.sfu.ca/projects/IntegerRelations`

8. The CECM inverse symbolic calculator (ISC):
   `http://oldweb.cecm.sfu.ca/projects/ISC`

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

10. The Dalhousie University inverse symbolic calculator version 2 (ISC2):
    `http://ddrive.cs.dal.ca/~isc`

11. The FFTW site (FFT software):
    `http://www.fftw.org`

12. The FIZ-Karlsruhe journal and abstract database:
    `http://www.zentralblatt-math.org/portal/en`

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://crd.lbl.gov/~dhbailey/mpdist`

15. The LBNL Experimental Mathematician's Toolkit:
    `http://crd.lbl.gov/~dhbailey/mpdist`

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

17. The LinBox symbolic linear algebra software library:
    `http://www.linalg.org/linbox-html/index.html`

18. The *Magma* computational algebra system:
    `http://magma.maths.usyd.edu.au/magma`

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

20. PSU's CiteSeer database:
    `http://citeseer.ist.psu.edu`

21. The Research Institute for Symbolic Computation (RISC) website:
    `http://www.risc.uni-linz.ac.at/research/combinat/software`

22. Neil Sloane's online dictionary of integer sequences:
    `http://www.research.att.com/~njas/sequences`

Other Sites of Interest

1. Abramowitz and Stegun's Handbook of Mathematical Functions (67 Mbyte; scanned copy courtesy Simon Plouffe; not subject to copyright):
   `http://www.experimentalmath.info/othersites/Abramowitz&Stegun.pdf`

2. David Anderson's decimal pi search facility:
   `http://www.angio.net/pi/piquery`

3. David Bailey's pi pages:
   `http://crd.lbl.gov/~dhbailey/pi`

4. Lee Borrell's "Absolute Certainty?" site:
   `http://www.fortunecity.com/emachines/e11/86/certain.html`

5. Jonathan Borwein's π pages:
   `http://oldweb.cecm.sfu.ca/personal/jborwein/pi_cover.html`

6. The CECM π recital site (recites π in numerous languages):
   `http://oldweb.cecm.sfu.ca/pi/yapPing.html`

7. Gregory Chaitin's site on algorithmic information theory:
   `http://www.cs.umaine.edu/~chaitin`

8. Ivan Cnop's Exploot site:
   `http://we.vub.ac.be/exploot/summary.html`

9. The de Smit-Lenstra site on the mathematics of Escher's "Print Gallery":
   `http://escherdroste.math.leidenuniv.nl`

10. Stewart Dickson's math art site:
    `http://emsh.calarts.edu/~mathart`

11. The electronic geometry site:
    `http://www.eg-models.de`

12. The Embree-Trefethen-Wright pseudospectra and eigenproblem site:
    `http://web.comlab.ox.ac.uk/projects/pseudospectra`

13. Helaman Ferguson's mathematical sculpture site:
    `http://www.helasculpt.com`

14. Steven Finch's mathematical constant site:
    `http://pauillac.inria.fr/algo/bsolve/constant/constant.html`

15. The Geometry Analysis Numerics Graphics (GANG) site:
    `http://www.gang.umass.edu`

16. Xavier Gourdon and Pascal Sebah's site for famous math constants:
    `http://numbers.computation.free.fr/Constants/constants.html`

17. Andrew Granville's Pascal triangle site:
    `http://www.cecm.sfu.ca/organics/papers/granville/support/pascalform.html`

18. David Griffeath's cellular automata site:
    `http://psoup.math.wisc.edu`

19. Jerry Grossman's Erdős number site:
    `http://www.oakland.edu/enp/`

20. Thomas Hales' Kepler problem site:
    `http://www.math.pitt.edu/~thales/kepler98`

21. David Joyce's site (Java implementation of Euclid's *Elements*, and
    the Mandelbrot and Julia set explorer):
    `http://aleph0.clarku.edu/~djoyce`

22. Yasumasa Kanada's π site:
    `http://www.super-computing.org`

23. Leonard Lewin's listing of polylogarithm formulas (7 Mbyte; taken
    from *P*olylogarithms and Associated Functions, with permission):
    `http://www.experimentalmath.info/othersites/Lewin-polylog.pdf`

24. The mathpages.com site (various interesting notes about mathematics):
    `http://www.mathpages.com`

25. The Mersenne prime site:
    `http://www.mersenne.org`

26. National Institute of Standards and Technology's *Digital Library of
    Mathematical Functions*:
    `http://dlmf.nist.gov`

27. The Organic Mathematics Project site:
    `http://www.cecm.sfu.ca/organics`

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

29. George Reese's Buffon needle site:
    `http://www.mste.uiuc.edu/reese/buffon/buffon.html`

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

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

32. The Science Lab's mathematics site:
    `http://www.the-science-lab.com/Math`

33. Rob Scharein's KnotPlot research and development site:
    `http://www.colab.sfu.ca/KnotPlot`

34. Angela Vierling's mathematical models site:
    `http://math.bu.edu/people/angelav/projects/models`

35. Jeff Weeks' topology and geometry site:
    `http://www.geometrygames.org`

36. Figure 1.7 shows a Sierpinski cube plotted in *JavaView*
    `http://oldweb.cecm.sfu.ca/news/coolstuff/JVL/htm/gallery.htm`
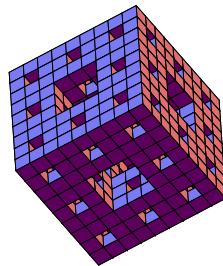
Figure 1.7. The Sierpinski cube.

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` and `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 [128]:

   > 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."[154, 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* [160], 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`

> 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` and `http://www.fortunecity.com/emachines/e11/86/certain.html`.

6. **Goodstein's theorem.** Another very striking example is that of *Goodstein sequences* [260]. 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

$$
\begin{aligned}
266_0 &= 266 \\
266_1 &= 3^{3^{3+1}} + 3^{3+1} + 2 \\
266_2 &= 4^{4^{4+1}} + 4^{4+1} + 1 \\
266_3 &= 5^{5^{5+1}} + 5^{5+1} \\
266_4 &= 6^{6^{6+1}} + 6^{6+1} - 1 \\
&= 6^{6^{6+1}} + 5 \cdot 6^6 + 5 \cdot 6^5 + \cdots + 5 \cdot 6 + 5 \\
266_5 &= 7^{7^{7+1}} + 5 \cdot 7^7 + 5 \cdot 7^5 + \cdots + 5 \cdot 7 + 4 \\
&\quad \cdots
\end{aligned}
$$

Done generally, this determines the *Goodstein sequence* starting at n. That is, we recursively define nonnegative integers $n_0 = n, n_1, \cdots, n_k, \ldots$ 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 $k = 3\left(2^{402653211} - 1\right) \approx 10^{121210695}$.

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 [188].

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

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`.

The *Annals of Mathematics* originally decided to publish Hales' paper with a cautionary note that although a team of referees is "99% certain" that the computer-assisted proof is sound, they have not been able to verify every detail [271]. But the paper eventually appeared without the disclaimer.

8. **"That's Mathematics"**(© Tom Lehrer 1995, used by permission) in song.

1. Counting sheep	2. When a ball
When you're trying to sleep,	Bounces off of a wall,
Being fair	When you cook
When there's something to share,	From a recipe book,
Being neat	When you know
When you're folding a sheet,	How much money you owe,
That's mathematics!	That's mathematics!

3. How much gold can you hold in	4. When you choose
an elephant's ear?	How much postage to use,
When it's noon on the moon,	When you know
then what time is it here?	What's the chance it will snow,
If you could count for a year,	When you bet
would you get to infinity,	And you end up in debt,
Or somewhere in that vicinity?	Oh try as you may,
	You just can't get away
	From mathematics!

5. Andrew Wiles gently smiles,	6. Tap your feet,
Does his thing, and voila!	Keepin' time to a beat
Q.E.D., we agree,	Of a song
And we all shout hurrah!	While you're singing along,
As he confirms what Fermat	Harmonize
Jotted down in that margin,	With the rest of the guys,
Which could've used some enlargin'.	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... and rotated clockwise by 157.6255960832... degrees [126]. This research received feature coverage in the *New York Times* [245]. 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)

11. **Gravitational boosting.** "The Voyager Neptune Planetary Guide" (JPL Publication 89–24) has an excellent description of Michael Minovitch's computational and unexpected discovery of gravitational boosting (otherwise known as slingshot magic) at the Jet Propulsion Laboratory in 1961.

    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 set of points in four dimensional space at unit distance from the
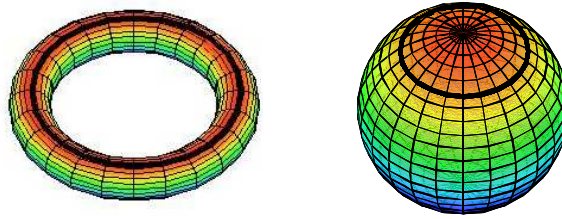
Figure 1.8. The torus and the two-sphere.

origin). This question turned out to be extraordinarily difficult,
and mathematicians have been struggling with it ever since.

Peter Sarnak, a well-known Princeton University mathematician, de-
scribed Perelman's work in these words: "He's not facing Poincaré
directly, he's just trying to do [a] grander scheme." The Poincaré re-
sult 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 math-
ematics; the dream of every mathematician" [97]. Along this line, a
New York Times report [176] 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 $a_1, a_2, \cdots, a_n$, 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" [165]. 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 [217].

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 [167, 168], 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 [64].)

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* [198, 179])

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.

(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." [160, 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 [210, 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."

(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 [148, 206]:

> 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 [185, 206]:

> 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 [206]:

> Ericsson and Charness [136] 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.

2 | Experimental Mathematics in Action

The purpose of computing is insight, not numbers.

> – Richard Hamming, *Numerical Methods for Scientists and Engineers*, 1962

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

$$\binom{m}{n}$$

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,

$$\binom{m}{n} \quad = \quad \frac{m!}{n!(m-n)!}, \tag{2.1}$$

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

$$F_2(m,n) \quad = \quad \binom{m}{n} \bmod 2. \tag{2.2}$$

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

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

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

where $B_1(m)$ is the number of 1s in the binary representation of m [152].

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. 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 [213]. In fact, it can be seen that this figure exhibits the fractional dimension $\log_2 3 = 1.58496 \ldots$ [289].

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 associated with each one in the binary expansion of m. This proves (2.3).
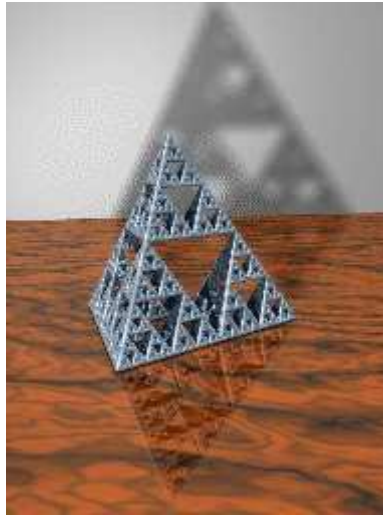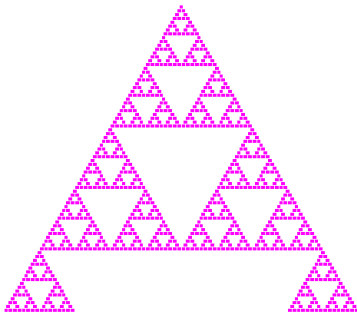
Figure 2.1. Pascal triangles modulo two? (see Color Plate I.) Courtesy of Daryl Hepting.

See Stephen Wolfram's article [289] and the Crandall-Pomerance book [118] (research problem 8.22) for additional details and some generalizations.

We should add here that Wolfram has recently published his long-awaited tome *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 [290].

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:

$$(x', y') \quad = \quad \left(\frac{1}{2}(x + x_r), \frac{1}{2}(y + y_r) \right). \qquad (2.4)$$

This procedure is then iterated indefinitely.
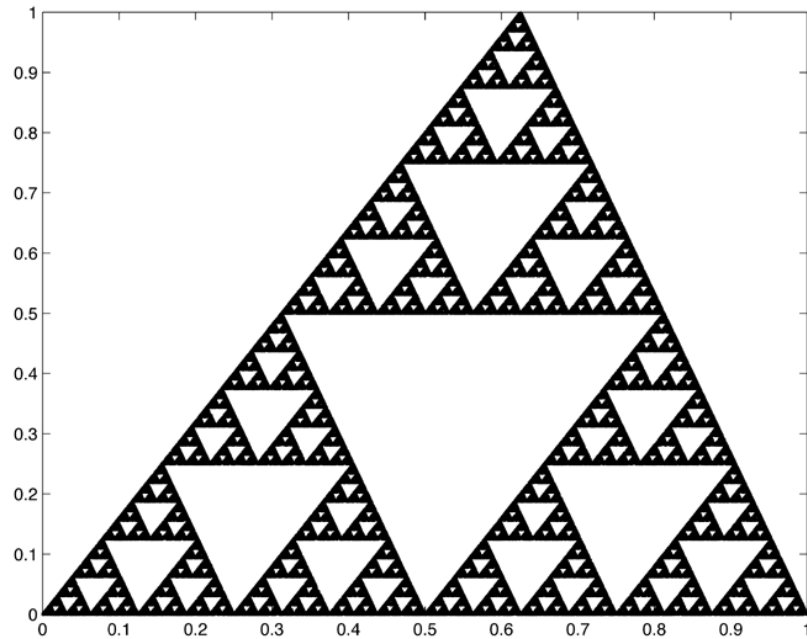
Figure 2.2. Sierpinski triangle by random selections.

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* [44].

2.2   A Curious Anomaly in the Gregory Series

In 1988, Joseph Roy North of Colorado Springs observed that Gregory's series for π,

$$\pi \;=\; 4\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{2k-1} \;=\; 4(1-1/3+1/5-1/7+\cdots), \qquad (2.5)$$

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

```
3.141592453589793238464643383279502784197169399387305820974941822230781640...
3.141592653589793238464264338327950288419716939937510582097494459230781640...
       2              -2            10           -122          2770
```

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 π. 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 $\log 2 = 1 - 1/2 + 1/3 - 1/4 + \cdots$ shows:

```
0.6931470805599553094172321212581765680755161343602552514000680000949418722...
0.6931471805599945309417232121458176568075500134360255254120680000949339362...
          1      -1           2          -16           272          -7936
```

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 $(1, -1, 5, -122, 1385)$.

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. 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:

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

$$\tan x = \sum_{k=0}^{\infty} \frac{(-1)^{k+1} T_{2k+1} x^{2k+1}}{(2k+1)!}. \tag{2.6}$$

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:

$$\frac{\pi}{2} - 2\sum_{k=1}^{N/2} \frac{(-1)^{k+1}}{2k-1} \approx \sum_{m=0}^{\infty} \frac{E_{2m}}{N^{2m+1}} \tag{2.7}$$

$$\log 2 - \sum_{k=1}^{N/2} \frac{(-1)^{k+1}}{k} \approx \frac{1}{N} + \sum_{m=1}^{\infty} \frac{T_{2m-1}}{N^{2m}}. \tag{2.8}$$

Now the genesis of the anomaly mentioned above is clear: North, in computing π 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 π. And the asymptotic expansions show up on the computer screen, as we observed above. Similar phenomena occur for other constants. (See [69] 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

$$x_{k+1} = r x_k (1 - x_k). \tag{2.9}$$
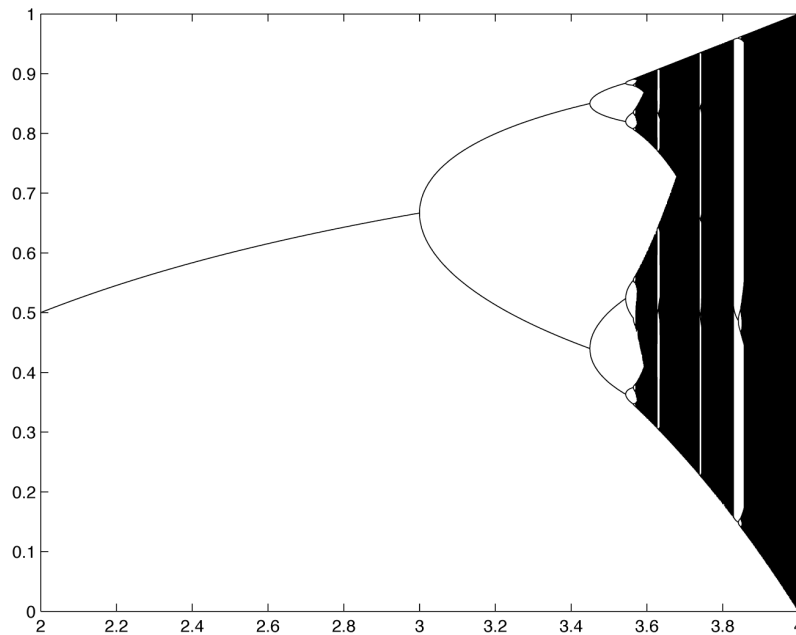
Figure 2.3. Bifurcation in the logistic iteration.

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 $a_1 x_1 + a_2 x_2 + \cdots + a_n x_n = 0$ (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 [139, 18, 35], 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 http://oldweb.cecm.sfu.ca/projects/IntegerRelations and the Experimental Mathematician's Toolkit at 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 α, 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 α.

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

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

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
    5303058429 4285886301 2256258566 4248917999 6260899277 5899745457

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

```
FindRoot[4913 + 2108*t^2 - 604*t^3 - 977*t^4 + 8*t^5
    + 44*t^6 + 392*t^7 - 193*t^8 - 40*t^9 + 48*t^10 - 12*t^11
    + t^12 == 0, {t, 3.544}, WorkingPrecision -> 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 [35]. The relation produced was recently verified by Konstantinos Karamanos, using the Magma computer algebra system [190].

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 [147]. 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 [88].

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* [18]. 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 [138]. 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." [236]

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 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 32 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 32 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

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

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

In 1998, British physicist David Broadhurst conjectured that $V/\sqrt{3}$ is a rational linear combination of

$$C_j = \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n(6n+j)^2}. \tag{2.13}$$

Indeed, it is, as Broadhurst [93] found using a PSLQ program:

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

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:

```
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 33 and 34. 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 [65]

$$\sum_{k=1}^{\infty} \left(1 + \frac{1}{2} + \cdots + \frac{1}{k} \right)^2 k^{-2} = 4.59987\ldots$$

$$\approx \frac{17}{4}\zeta(4) = \frac{17\pi^4}{360}. \tag{2.15}$$

The function $\zeta(s)$ in (2.15) is the classical *Riemann zeta function*,

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

Euler showed that for even integers, $\zeta(2n)$ is a rational multiple of π^{2n} [74]. (Euler'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

$$\frac{1}{2\pi} \int_0^\pi (\pi - t)^2 \log^2\!\Big(2\sin\frac{t}{2}\Big)\, dt \;\; = \;\; \sum_{n=1}^\infty \frac{(\sum_{k=1}^n \frac{1}{k})^2}{(n+1)^2}. \qquad (2.16)$$

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, $17/360 = 0.047222\ldots$ 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 [130]. 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

$$\sum_{k=1}^\infty \left(1 + \frac{1}{2^m} + \cdots + \frac{1}{k^m}\right)(k+1)^{-n}. \qquad (2.17)$$

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 [31]) found a satisfactory scheme involving the Euler-Maclaurin summation formula. Another, more powerful scheme is described in [67]. 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 [66]. 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.

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

$$\sum_{k=1}^{\infty} \left(1 + \frac{1}{2} + \cdots + \frac{1}{k}\right)^3 (k+1)^{-6} \;\; =$$

$$\zeta^3(3) + \frac{197}{24}\zeta(9) + \frac{1}{2}\pi^2\zeta(7) - \frac{11}{120}\pi^4\zeta(5) - \frac{37}{7560}\pi^6\zeta(3),$$

$$\sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \cdots + (-1)^{k+1}\frac{1}{k}\right)^2 (k+1)^{-3} \;\; =$$

$$4\operatorname{Li}_5\left(\frac{1}{2}\right) - \frac{1}{30}\log^5(2) - \frac{17}{32}\zeta(5) - \frac{11}{720}\pi^4\log(2) + \frac{7}{4}\zeta(3)\log^2(2)$$

$$+ \frac{1}{18}\pi^2\log^3(2) - \frac{1}{8}\pi^2\zeta(3), \tag{2.18}$$

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

2.6   Quantum Field Theory

In another recent development, David Broadhurst (who discovered the iden-
tity (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 [95, 96]. 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
[93], 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 $\omega_k = dx/(\lambda^{-k} - x)$, where $\lambda = (1+\sqrt{-3})/2$ is the primitive
sixth root of unity, and k runs from 0 to 5. A four-letter word here is a
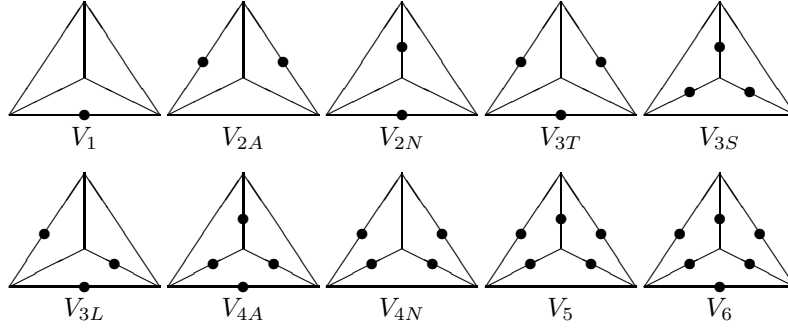
Figure 2.6. The ten tetrahedral configurations.

four-dimensional iterated integral, such as

$$U = \zeta(\Omega^2\omega_3\omega_0) =$$
$$\int_0^1 \frac{dx_1}{x_1} \int_0^{x_1} \frac{dx_2}{x_2} \int_0^{x_2} \frac{dx_3}{(-1-x_3)} \int_0^{x_3} \frac{dx_4}{(1-x_4)} = \sum_{j>k>0} \frac{(-1)^{j+k}}{j^3 k}.$$

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

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

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

$$
\begin{aligned}
V_1 &= 6\zeta(3) + 3\zeta(4) \\
V_{2A} &= 6\zeta(3) - 5\zeta(4) \\
V_{2N} &= 6\zeta(3) - \tfrac{13}{2}\zeta(4) - 8U \\
V_{3T} &= 6\zeta(3) - 9\zeta(4) \\
V_{3S} &= 6\zeta(3) - \tfrac{11}{2}\zeta(4) - 4C^2 \\
V_{3L} &= 6\zeta(3) - \tfrac{15}{4}\zeta(4) - 6C^2 \\
V_{4A} &= 6\zeta(3) - \tfrac{77}{12}\zeta(4) - 6C^2 \\
V_{4N} &= 6\zeta(3) - 14\zeta(4) - 16U \\
V_5 &= 6\zeta(3) - \tfrac{469}{27}\zeta(4) + \tfrac{8}{3}C^2 - 16V \\
V_6 &= 6\zeta(3) - 13\zeta(4) - 8U - 4C^2
\end{aligned}
$$

Table 2.1. Formulas found by PSLQ for the ten tetrahedral diagrams.

following three integrals to over 100 decimal digit accuracy:

$$\int_0^1 \frac{t^2 \log(t)\ dt}{(t^2 - 1)(t^4 + 1)} =$$

0.180671262590654942792308128981671615337114571018296766266240794293758566224133001770898254150483799707740 . . .

$$\int_0^{\pi/4} \frac{t^2\ dt}{\sin^2(t)} =$$

0.843511841685034634002620051999528151651689086421444293697112596906587355669239938399327915596371348023976 . . .

$$\int_0^{\pi} \frac{x \sin x\ dx}{1 + \cos^2 x} =$$

2.467401100272339654708622749969037783828424851810197656603337344055011205604801310750443350929638057956006 . . .   (2.19)

(the third of these is from [157]). 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.ddrive.cs.dal.ca/~isc, we obtain the following, based solely on the numerical values above:

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

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

$$\int_0^{\pi} \frac{x \sin x\ dx}{1 + \cos^2 x} = \frac{\pi^2}{4}, \qquad (2.20)$$

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 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

$$\int_0^{\pi/4} \frac{t^3 \, dt}{\sin^2(t)}.$$

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 π. 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

$$\pi = 48 \arctan \frac{1}{49} + 128 \arctan \frac{1}{57} - 20 \arctan \frac{1}{239} + 48 \arctan \frac{1}{110443}$$

$$\pi = 176 \arctan \frac{1}{57} + 28 \arctan \frac{1}{239} - 48 \arctan \frac{1}{682} + 96 \arctan \frac{1}{12943}.$$
$$\tag{2.21}$$

One way to do this is by using the "Experimental Mathematician's Toolkit," which is available at http://www.experimentalmath.info. Type the string

```
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 π 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 [151]. They were studying the sequences (a_n) and (b_n), defined by $a_0 = m$, then

$$a_{n+1} = \lfloor \sqrt{2a_n(a_n + 1)} \rfloor \tag{2.22}$$

followed by

$$b_n = a_{2n+1} - 2a_{2n-1}. \tag{2.23}$$

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 $m \geq 1$,

$$\alpha(m) \quad = \quad 0.b_1 b_2 b_3 \cdots_2, \qquad (2.24)$$

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,

$$
\begin{aligned}
\alpha(1) &= \sqrt{2} - 1 \\
\alpha(2) &= \sqrt{2} - 1 \\
\alpha(3) &= 2\sqrt{2} - 2 \\
\alpha(4) &= 2\sqrt{2} - 2 \\
\alpha(5) &= 3\sqrt{2} - 4 \\
\alpha(6) &= 4\sqrt{2} - 5 \\
\alpha(7) &= 3\sqrt{2} - 4 \\
\alpha(8) &= 5\sqrt{2} - 7 \\
\alpha(9) &= 4\sqrt{2} - 5 \\
\alpha(10) &= 6\sqrt{2} - 8.
\end{aligned}
$$

This recognition led to an explicit formula for the sequence (a_n) as

$$a_n \quad = \quad \lfloor \tau(2^{(n-1)/2} + 2^{(n-2)/2}) \rfloor, \qquad (2.25)$$

where τ 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 [151] for complete details. It is not known if generalized sequences such as

$$a_{n+1} \quad = \quad \lfloor \sqrt{3a_n(a_n + 1)} \rfloor \qquad (2.26)$$

$$a_{n+1} \quad = \quad \lfloor \sqrt[3]{2a_n(a_n + 1)(a_n + 2)} \rfloor \qquad (2.27)$$

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 $\int_2^x dt/\log t$. [153, 149]

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 [118]. 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 π:

> 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. [144, 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. [292]

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 [118], 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 [153].

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

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

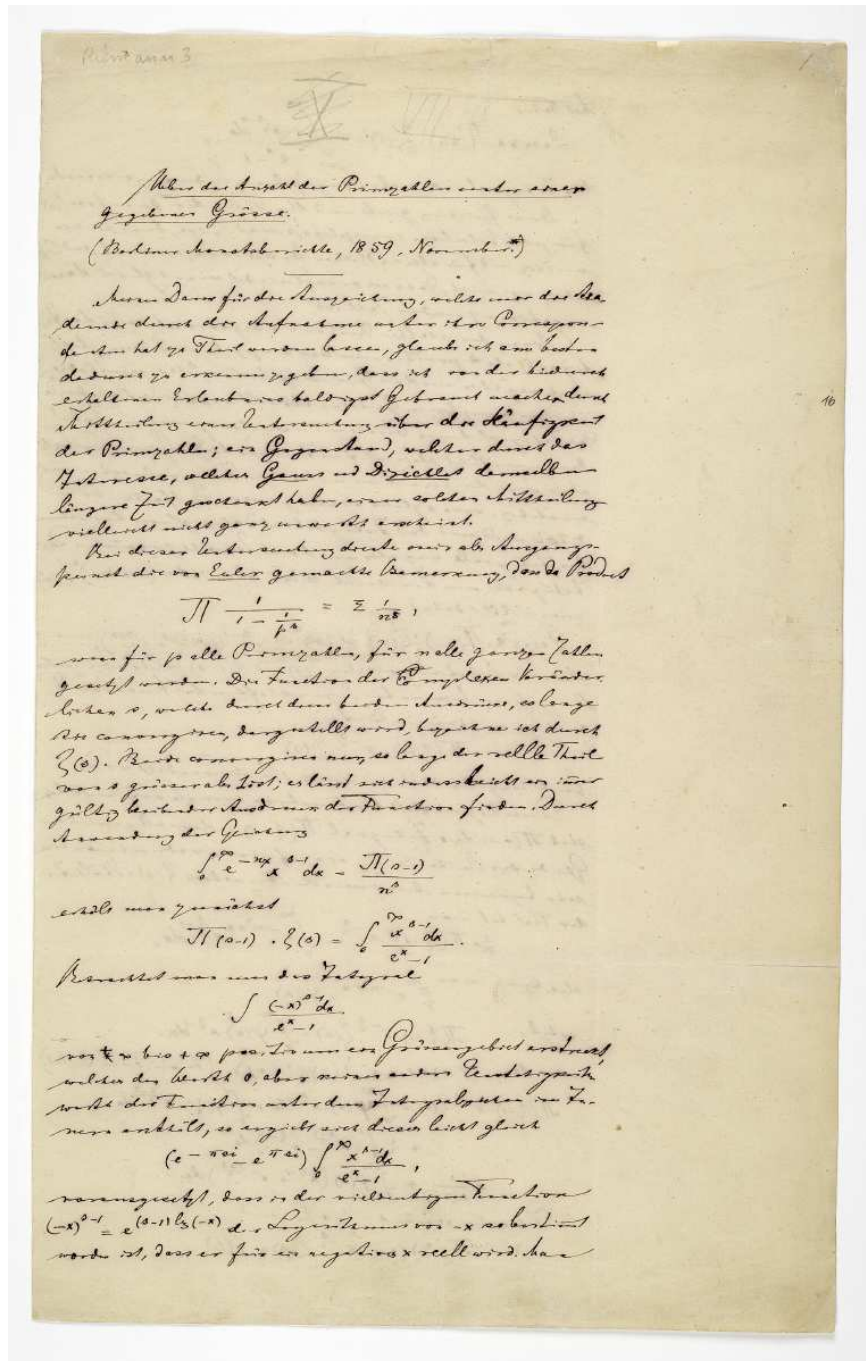Table 2.2. The prime-counting function $\pi(x)$ and Gauss' approximation.

Figure 2.7. Page 1 of Riemann's 1859 manuscript. Courtesy of Nieder-sächsische Staats- und Universitätsbibliothek Göttingen.
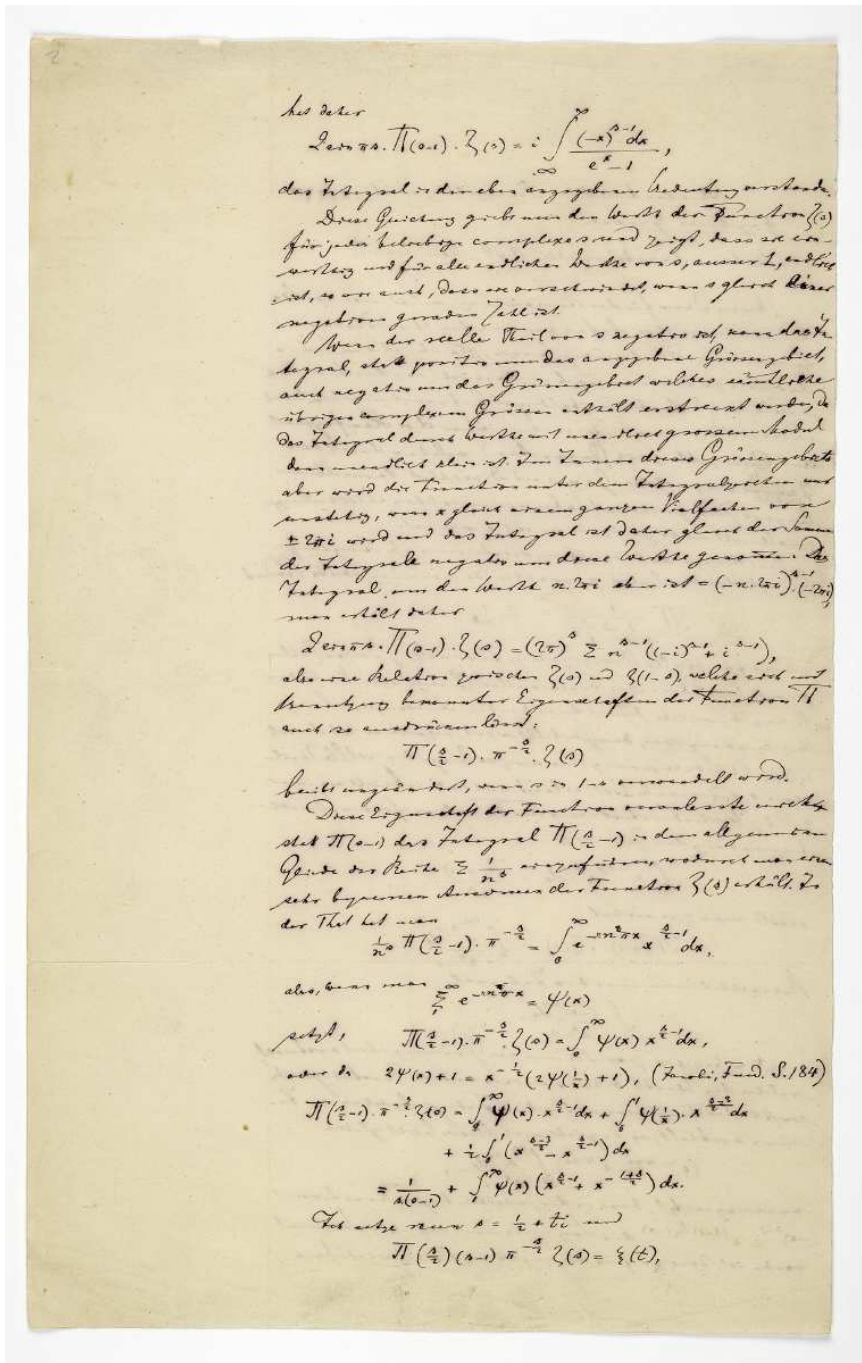
Figure 2.8. Page 2 of Riemann's 1859 manuscript. Courtesy of Niedersächsische Staats- und Universitätsbibliothek Göttingen.

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 (on the Riemann hypothesis) that the first sign change must occur at least by $10^{10^{10^{34}}}$, a number known as the *Skewes number* because of its prodigious size (see [118], Exercise 1.35). This bound has recently been reduced to a "tiny" number, a mere 10^{316} [153]. Littlewood [203, 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

$$\frac{\pi(x) - \int_2^x dt/\log t}{\sqrt{x}/\log x} \quad \approx \quad -1 - 2\sum_{\gamma \in S} \frac{\sin(\gamma \log x)}{\gamma}, \qquad (2.28)$$

where S is the set of γ such that $\gamma > 0$ and $1/2 + i\gamma$ is a zero of the analytic continuation 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 $0 \le \sigma \le 1$ are for $\sigma = 1/2$ [242]. 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" [153]. 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 $X_3, X_4, \cdots$ 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

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

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

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

(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 $144176897509546973538.498\ldots$), 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." [208]

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
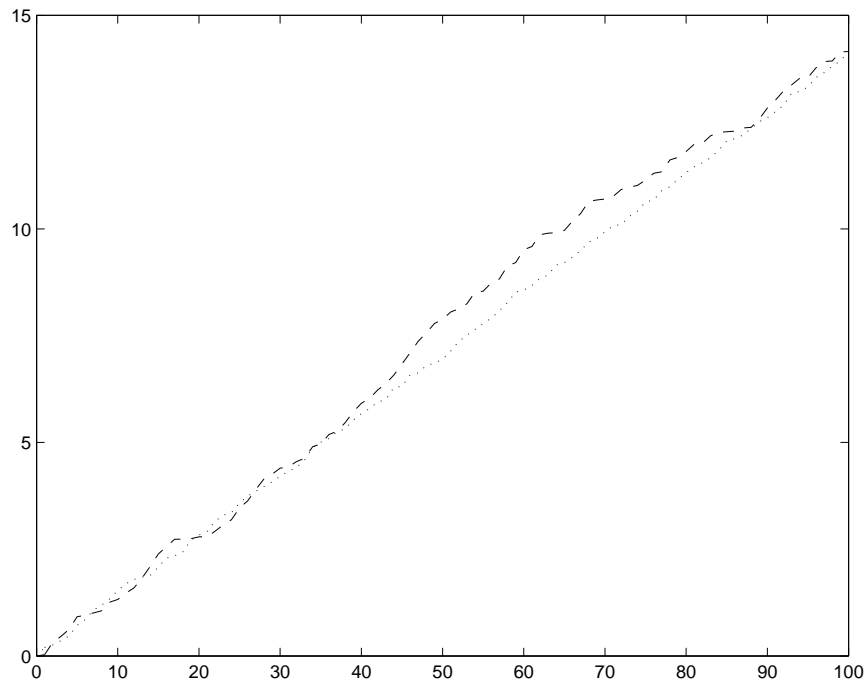
Figure 2.9.   Zeta function zeroes (dotted) vs pseudo-random data (dashed).

in a gap of length T times the average gap, following a zero, is

$$\int_0^T \left(1 - \left(\frac{\sin \pi u}{\pi u}\right)^2\right) du. \tag{2.31}$$

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 [224]. Figure 2.10 shows this spacing data based on a billion zeroes near the 1.3×10^{16}-th zero.
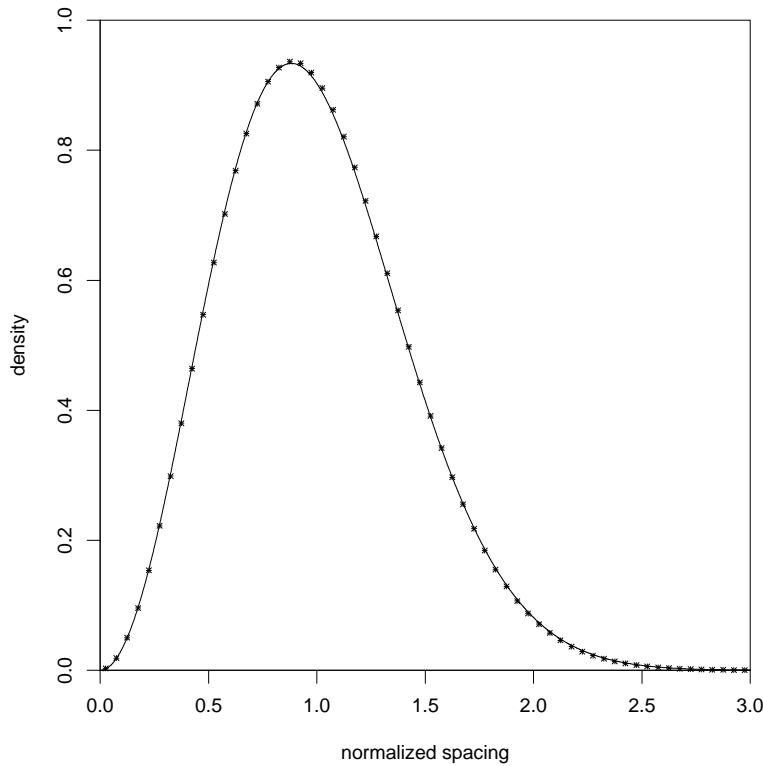
Nearest neighbor spacings

Figure 2.10. Nearest neighbor spacing versus Montgomery's distribution.

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 encoun-
tered 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 serendipitious 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) [249]. Then in 1996, two math-
ematical 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 [55]. 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. [186]

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 out-
standing mathematical problems) by the Clay Mathematics Institute. De-
tails of this prize are available on the Clay Institute web site http://www.claymath.org.
A very readable recent survey is to be found in [110].

2.9   Two Observations about $\sqrt{2}$

As we observed earlier in the discussion of Pascal's triangle, it is still pos-
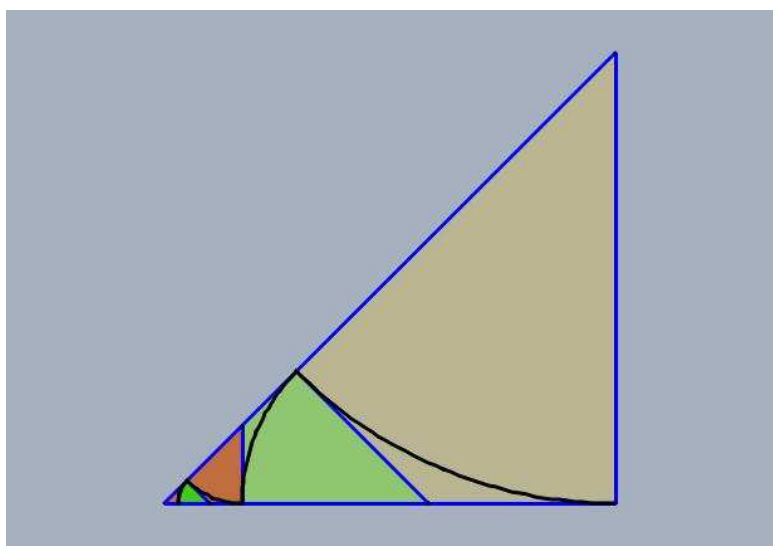sible to find new insights even in the oldest areas of mathematics. We

Figure 2.11. Root two is irrational (see Color Plate II).

illustrate this principle again with two intriguing observations on that oldest of irrational constants, the square root of two.

2.9.1   Irrationality

We first present Tom Apostol's lovely new geometric proof of the irrationality of $\sqrt{2}$ [9].

Proof.   To say $\sqrt{2}$ is rational is to draw a right-angled isoceles triangle with integer sides. Consider the *smallest* right-angled isoceles 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* isoceles 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 $p/q = \sqrt{n}$, then

$$\frac{p'}{q'} \;=\; \frac{n\,q - \lfloor\sqrt{n}\rfloor\,p}{p - \lfloor\sqrt{n}\rfloor\,q} \;=\; \frac{p}{q} \tag{2.32}$$

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:

$$\left(\sqrt{2}^{\sqrt{2}}\right)^{\sqrt{2}} \;=\; \sqrt{2}^{\left(\sqrt{2}\cdot\sqrt{2}\right)} \;=\; \sqrt{2}^{\,2} = 2. \tag{2.33}$$

Hence, by the *principle of the excluded middle*,

$$\text{either } \sqrt{2}^{\sqrt{2}} \in \mathbf{Q} \text{ or } \sqrt{\mathbf{2}}^{\sqrt{\mathbf{2}}} \notin \mathbf{Q}.$$

In either case, we can deduce that there are irrational numbers α and β with α^β 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 27), 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 28). 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) [278]:

> [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 ℓ_n of $\sigma_n = \sum_{k=1}^{n} k$. (Taken from [157]).

   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 (see also [197]), with records stored at 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

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

   Answer: $\mathcal{K} = \sqrt{\pi} e^{-3970}/\sqrt{1985}$. The Putnam problems listed here and in subsequent chapters are taken from [184]. *Hint*: This is problematic to evaluate numerically as stated, since its value is tiny. So

consider instead $\mathcal{K}(\alpha) = \int_0^\infty t^{-1/2} e^{-\alpha(t+t^{-1})} \, dt$ for some other specific (or general) constant α.

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

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

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

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

for $0 \le y \le 1$. *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 $n \ge 0$. 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 a 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.

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

$$\sigma = \sqrt[8]{2207 - \cfrac{1}{2207 - \cfrac{1}{2207 - \cfrac{1}{2207 - \cdots}}}}. \qquad (2.34)$$

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 $\sigma^4 + \sigma^{-4} = 47$. Answer: $(3 + \sqrt{5})/2$.

13. **Berkeley problem 1.1.35.** Find the derivative at $x = 0$ of

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

Hint: Plot it. Answer $= (e - 3)/2$. The Berkeley problems listed here and in subsequent chapters are taken from [127].

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 [166, 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: $\sqrt[3]{\frac{1}{2}(5 - 3\sqrt[3]{7})}$ and $\sqrt[3]{\frac{3}{2}\sqrt[3]{9} - 3/2}$.

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 π^e.

17. **Crandall's continued fraction.** Compute, then guess and prove, the continued fraction for

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

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

$$11\,z^{10} + 10\,iz^9 + 10\,iz - 11 = 0$$

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 $(x^2 + y^2)^m = (xy)^n$. *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 $\sqrt{2} + \sqrt[3]{3}$ is irrational. *Hint*: Use *Maple* or *Mathematica* to find the minimum polynomial of this constant.

22. **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 [204]. It is still open [204].

23. **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 Césaro 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:*

$$3, 5, 7, \cdots 2\cdot3, 2\cdot5, 2\cdot7, \cdots 2^2 3, 2^2 5, 2^2 7, \cdots 2^3 3, 2^3 5, 2^3 7, \cdots, \cdots, 2^3, 2^2 2, 2, 1.$$

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

24. **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

$$Q_N = \sum_{n=0}^{\infty} \frac{n^n e^{-n}}{(n+N)!} - \sum_{k=1}^{N} \frac{(-1)^{k-1} e^k}{(N-k)!\, k^k} \qquad (2.35)$$

is a rational number. The first four are $-1, -1/4, -7/108, -97/6912$. Continuing in this manner, you can ultimately discover that

$$Q_N = \sum_{k=1}^{N} \frac{(-1)^k}{(N-k)!k^k} \sum_{n=0}^{k-1} \frac{k^n}{n!}. \qquad (2.36)$$

This relies on replacing $\exp(-n)$ by its series, exchanging order of summation, and then discovering and deriving the identity

$$\sum_{k=0}^{n}(-1)^k\,k^n\binom{N+n}{N+k}=(-1)^n\sum_{k=1}^{N}k^n(-1)^{k-1}\binom{N+n}{N-k}\quad(2.37)$$

or equivalently,

$$\sum_{k=0}^{M+N}(-1)^k\,(M-k)^M\binom{M+N}{k}\;=\;0\qquad\qquad(2.38)$$

for all $M, N > 0$. This in turn follows (using the binomial theorem) from

$$\sum_{k=0}^{P}(-1)^k\,k^n\binom{P}{k}\;=\;0,\qquad\qquad(2.39)$$

for all $0 \le n < P$. The final identity (2.39) is established by setting $Df(x) = xf'(x)$ and observing that $D^k(1-x)^P$ has a zero at 1 for $k < P$.

25. **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 [203]. More of Littlewood is to be found at the end of Chapter 4 of the second volume.

   (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 isoperimerical 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

$$\text{area} = \frac{1}{2}\int_0^{\frac{\pi}{2}}\left(r^2(\theta)+r^2(\theta-\frac{\pi}{2})\right)\,d\theta,$$
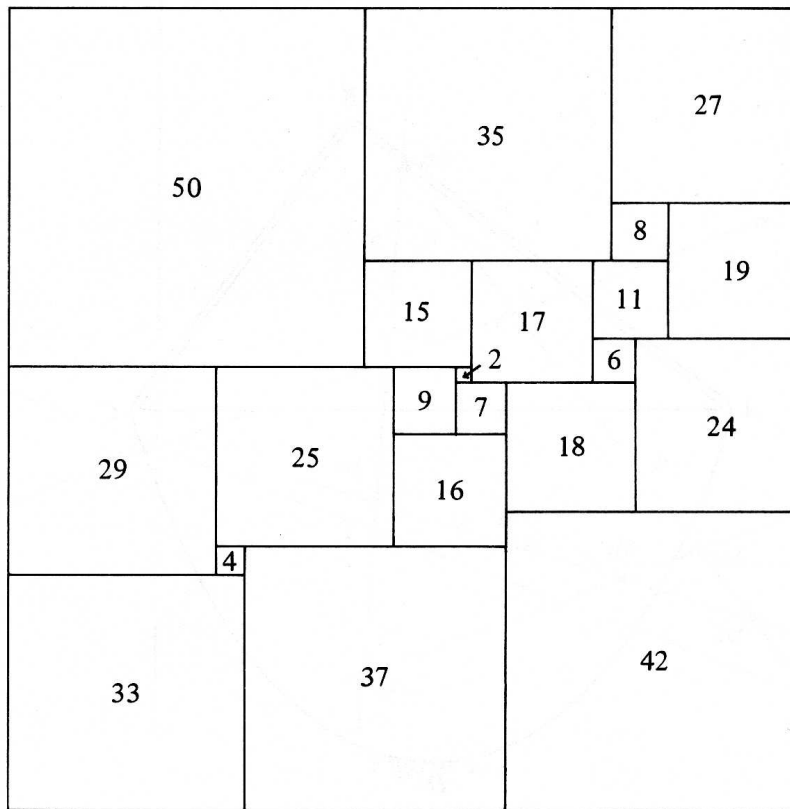
   and the integrand never exceeds one.

Figure 3

Figure 2.12. Duijvestijn's dissection. Courtesy of Bela Bollobas.

(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 ϵ the area swept can be less than ϵ."

(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,
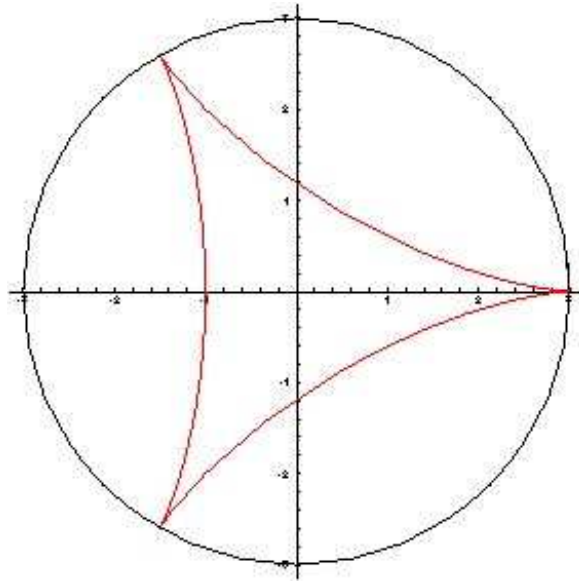
Figure 2.13. Kakeya's conjectured answer—the three-cusp hypocycloid.

H. Hardy'."

"A minute I wrote (about 1917) for the Ballistics office ended with the sentence 'Thus σ 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 σ I have ever seen (the printers must have scoured London for it.)."

26. **The hypocycloid.** Cartesian coordinates are given by

$$x = (a - b)\cos(t) + b\cos\left((a/b - 1)t\right),$$

$$y = (a - b)\sin(t) - b\sin\left((a/b - 1)t\right)$$

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.

27. **The Gelfond-Schneider theorem.** This is the result that for complex algebraic numbers $\alpha \neq 0, 1$ and β irrational, the quantity α^β is transcendental. It follows that

(a) $\sqrt{2}^{\sqrt{2}}$ is transcendental; and

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

28. **Eight solutions.** Find examples of all eight rational and irrational possibilities of $\alpha^{\beta} = \gamma$.

29. **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 [118].

30. **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 perfection such as only the greatest art can show. [250, pg. 73]

This quote is doubly interesting given the fact that Russell may have
been responsible for Coxeter pursuing a mathematical career, accord-
ing 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 sup-
porting Coxeter's nomination to receive an honorary doctorate at
York University in Toronto, Canada:

> Modern science is often driven by fads and fashion, and mathe-
> matics is no exception. Coxeter's style, I would say, is singularly
> unfashionable. He is guided, I think, almost completely by a

Figure 2.14. Donald Coxeter's own kaleidoscope (see Color Plate VII).
Courtesy of Asia Weiss.

Figure 2.15. The "Firmament" by John Robinson (see Color Plate VI). Courtesy of Asia Weiss.

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 accounted 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
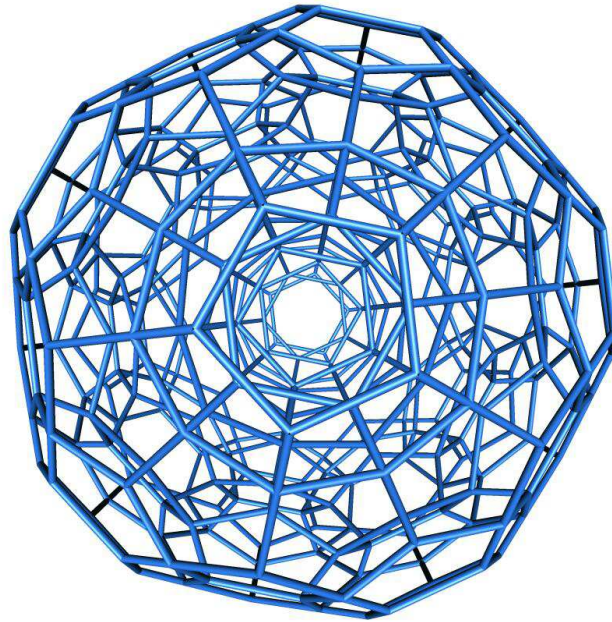
Figure 2.16. A projection of a four dimensional polytope (see Color Plate III).

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 and 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 $GL_n(Z)$. 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. [219]

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
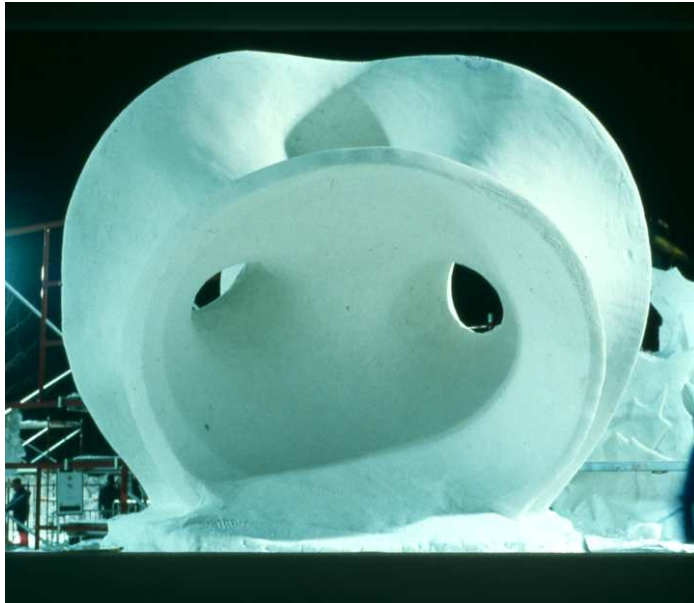
Figure 2.17. Ferguson's "Invisible Handshake" sculpture (see Color Plate V). Courtesy of Helaman Ferguson.

> 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. [285]

31. **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 [107]. 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.)

32. **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 2×2 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 Γ denote the multiplicative group of 2×2 matrices generated by the matrices

$$\begin{bmatrix} 1 & 0 \\ 0 & \omega_3 \end{bmatrix} \text{ and } \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \tag{2.40}$$

This Γ 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 $U_2 \backslash SL_2(C)$ is geometrically the three-dimensional hyperbolic space. This group Γ is an "arithmetic" subgroup of $SL_2(C)$. The group $SL_2(Z[\omega_3])$ 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 [276].

33. **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,

$$
\begin{aligned}
V &= \frac{2}{\sqrt{27}} \sum_{k=0}^{\infty} \left(\frac{-1}{27}\right)^k \left(\frac{9}{(6k+1)^2} - \frac{9}{(6k+2)^2} - \frac{12}{(6k+3)^2} \right. \\
&\quad \left. - \frac{3}{(6k+4)^2} + \frac{1}{(6k+5)^2}\right).
\end{aligned} \tag{2.41}
$$

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*

$$
V = -2 \int_0^{\pi/3} \log\left(2\sin\left(\frac{t}{2}\right)\right) dt \tag{2.42}
$$

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

$$
\mathrm{Cl}_2(\theta) = \sum_{n>0} \frac{\sin(n\theta)}{n^2}, \tag{2.43}
$$

which satisfies $\mathrm{Cl}_2(\frac{\pi}{2}) = G$. Then integration of (2.42) shows

$$
\begin{aligned}
V &= i\left\{\mathrm{Li}_2\left(e^{-i\pi/3}\right) - \mathrm{Li}_2\left(e^{i\pi/3}\right)\right\} \\
&= 2\,\mathrm{Im}\,\mathrm{Li}_2\left(\frac{1+i\sqrt{3}}{2}\right) = 2\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) = 3\,\mathrm{Cl}_2\left(\frac{2\pi}{3}\right).
\end{aligned}
$$

All the requisite details about Clausen's function are to be found in Lewin [201].

(b) A hypergeometric equivalent formulation of (2.41) is

$$
\begin{aligned}
\frac{V}{\sqrt{3}} &= 2\,F\left(\frac{1}{6},\frac{1}{6},1;\frac{7}{6},\frac{7}{6};\frac{-1}{27}\right) - \frac{1}{2}\,F\left(\frac{1}{3},\frac{1}{3},1;\frac{4}{3},\frac{4}{3};\frac{-1}{27}\right) \\
&\quad - \frac{8}{27}\,F\left(\frac{1}{2},\frac{1}{2},1;\frac{3}{2}\frac{3}{2};\frac{-1}{27}\right) - \frac{1}{24}\,F\left(\frac{2}{3},\frac{2}{3},1;\frac{5}{3},\frac{5}{3};\frac{-1}{27}\right) \\
&\quad + \frac{2}{225}\,F\left(\frac{5}{6},\frac{5}{6},1;\frac{11}{6},\frac{11}{6};\frac{-1}{27}\right)
\end{aligned}
$$

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

$$V \overset{?}{=} \mathrm{Im} \left\{ 4\,\mathrm{Li}_2 \left(\frac{i\sqrt{3}}{3} \right) - \frac{8}{3}\,\mathrm{Li}_2 \left(\frac{i\sqrt{3}}{9} \right) \right.$$

$$\left. + \mathrm{Li}_2 \left(\frac{1}{2} - \frac{i\sqrt{3}}{6} \right) + 8\,\mathrm{Li}_2 \left(-\frac{1}{2} + \frac{i\sqrt{3}}{6} \right) \right\}.$$

(c) Now, Lewin in Equation (5.5) of [201] gives

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

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

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

which is true by applying the two variable identities for Clausen's function given in Equations (4.61) and (4.63) of [201], with $\theta = \frac{\pi}{3}$.

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

$$6\,G = 2\,\mathrm{Cl}_2 (2\,\alpha) - 3\,\mathrm{Cl}_2 \left(2\,\alpha - \frac{\pi}{2} \right) + \mathrm{Cl}_2 \left(2\,\alpha + \frac{\pi}{2} \right).$$

A much harder identity is

$$\frac{7\sqrt{7}}{4}\,L_{-7} (2) \overset{?}{=} 3\,\mathrm{Cl}_2 (\alpha) - 3\,\mathrm{Cl}_2 (2\,\alpha) + \mathrm{Cl}_2 (3\,\alpha)$$

with $\alpha = 2\arctan\left(\sqrt{7}\right)$.

34. **Further identities for the knot complement volume.** These are explored below.

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

$$\begin{aligned} V &= \sum_{n \geq 1} \frac{2\sin(n\pi/3)}{n^2} \\ &= \sqrt{3} \left(\sum_{n=0}^{\infty} \frac{1}{(6n+1)^2} + \sum_{n=0}^{\infty} \frac{1}{(6n+2)^2} \right. \\ &\quad \left. - \sum_{n=0}^{\infty} \frac{1}{(6n+4)^2} - \sum_{n=0}^{\infty} \frac{1}{(6n+5)^2} \right), \end{aligned}$$

or equivalently,

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

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

$$V = -2 \int_0^1 \frac{\log(y)}{\sqrt{1 - \left(\frac{y}{2}\right)^2}} \, dy = 2 \sum_{n=0}^{\infty} \frac{\binom{2n}{n}}{(2n+1)^2 \, 16^n}.$$

The next two equivalent identities are derivable using (1.76) in [201] which gives the series for $\mathrm{Li}_2(e^{i\pi/3})$:

(c)

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

and

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

(d) Show that

$$V = 2\sqrt{3} \, \mathrm{Im} \, \mathrm{Li}_2\left(\frac{i\sqrt{3}+1}{2}\right) = -\sqrt{3} \int_0^1 \frac{\log y}{1 - y + y^2} \, dy.$$

(e) Hence expanding the last denominator and differentiating the β-function (see Section 5.4), deduce that

$$\begin{aligned} V &= \sqrt{3} \sum_{n \geq 1} \{\Psi(n) - \Psi(2n)\} \beta(n, n) = 2\sqrt{3} \sum_{n \geq 1} \frac{\sum_{k=n}^{2n-1} \frac{1}{k}}{n\binom{2n}{n}} \\ &= 2\sqrt{3} \sum_{n \geq 1} \frac{\sum_{k=1}^{2n-1} \frac{1}{k}}{n\binom{2n}{n}} - 2\sqrt{3} \sum_{n \geq 1} \frac{\sum_{k=1}^{n-1} \frac{1}{k}}{n\binom{2n}{n}}. \end{aligned}$$

(f) This is equivalent to

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

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

$$
\begin{aligned}
V &= \sqrt{3} \int_0^{\pi/2} \frac{\log\left(\frac{1+(\sin t)/2}{1-(\sin t)/2}\right)}{1-(\sin^2 t)/4}\, ds \\
&\quad -\sqrt{3} \int_0^{\pi/2} \left(\frac{-\sin t}{2}\right) \frac{\log(1-(\sin^2 t)/4)}{1-(\sin^2 t)/4}\, dt,
\end{aligned}
$$

where $\int_0^{\pi/2} \sin^{2N+1} t\, dt = \Gamma^2(N+1)4^N/\Gamma(2N+2)$, and $\int_0^{\pi/2} \sin^{2N} t\, dt = \Gamma^2(N+1/2)2^{2N-1}/\Gamma(2N+1)$. 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

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

(h) Finally,

$$
-\sqrt{3} \sum_{n=2}^{\infty} \frac{\sum_{k=1}^{n-1} k^{-1}}{n\binom{2n}{n}} = \frac{\sqrt{3}}{2} \int_0^1 \frac{\log(1-t(1-t))}{1-t+t^2}\, dt.
$$

Let

$$
H_1 = \sum_{n=1}^{\infty} \frac{\sum_{k=1}^{n-1} k^{-1}}{n\binom{2n}{n}}, \qquad H_2 = \sum_{n=1}^{\infty} \frac{\sum_{k=1}^{2n-1} k^{-1}}{n\binom{2n}{n}}.
$$

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

$$
\begin{aligned}
H_1 &= \sum_{k=0}^{\infty} \left(\frac{-1}{27}\right)^k \left\{ -\frac{1/3}{(6k+1)^2} + \frac{1}{(6k+2)^2} + \frac{10/9}{(6k+3)^2}\right. \\
&\quad \left. + \frac{1/3}{(6k+4)^2} - \frac{1/27}{(6k+5)^2}\right\},
\end{aligned}
$$

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 [201, 93] for additional details.

35. **Census of hypberbolic knots.** The URL http://newweb.cecm.sfu.ca/cgi-bin/KnotPlot/objtest/hyperbolic_c
contains
a census of hyperbolic knots (most, but not all, knots are hyper-
bolic). The figure-eight knot, not the trefoil, is now simplest when
viewed by the number of perfect tetrahedra in its complement.

36. **Jeff Weeks on experimental topology.** Jeff Weeks recently wrote:

> There are plenty of such [experimentally discovered topology] re-
> sults, 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).

Figure 2.18 attempts to illustrate Jeff Weeks' beautiful discovery.

37. **Griffeath's "psoup" cellular automata web site.** David Grif-
feath well describes his site 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 *Nonlin-
> ear Science Today* and *Scientific American.* Some of my cellu-
> lar 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
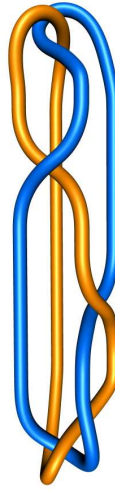> your own.

Figure 2.18. Weeks' two-bridge discovery.

> It's tempting to think of self-organization as evolution from pri-
> mordial soup. Machines that orchestrate such dynamics are
> sometimes called mixmasters. I use both garden-variety PCs
> and dedicated Cellular Automaton Machines (CAMs) as mix-
> masters. Since my other great fixation in life is gastronomy
> (witness the important 3-letter word hidden in my Welsh last
> name), this site is laid out as a kitchen.

38. **Fractal cards.** Not all impressive representations require a com-
puter. Elaine Simmt and Brent Davis [259] describe lovely construc-
tions made by repeated paper folding and cutting that result in beau-
tiful 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 similar-
ity to the tetrahedron in Figure 2.1. Recursive *Maple* code is given
below:

```
 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),
```
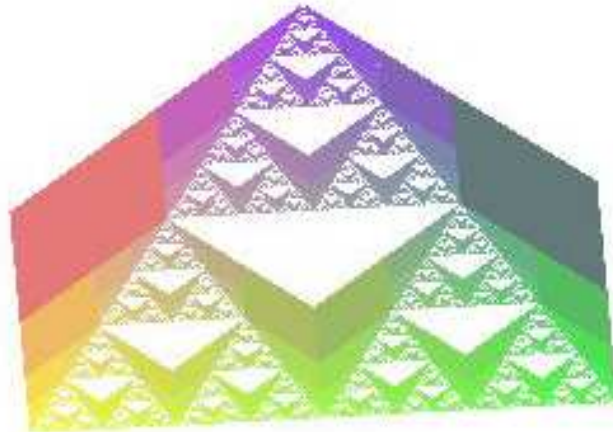
Figure 2.19. 7th iterate of Sierpinski triangle made by paper cutting and folding.

```
      AXESSTYLE(NONE), STYLE(PATCHNOGRID), ORIENTATION(90,45) );
   end:

   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:
```

39. **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. [265, 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, signally in chemistry, physics and astronomy, has been enormous.

40. **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 [110].

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 $Z(\cdot, y)$ implies the Riemann Hypothesis. This conclusion is given in [295], and was discovered while the first author of that paper was teaching an undergraduate complex variable class.

41. **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.

42. **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. [225]

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

43. **Tea with John-Paul II.** James Glanz wrote in "Web Archive Opens
a New Realm of Research" (*New York Times*, April 30, 2001):

> Three years ago, said Dr. Zanelli in Chile, one of his own stu-
> dents posted a paper and the next day received an e-mail mes-
> sage 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 with-
standing.

44. **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 Hy-
pothesis, the Four Color Theorem, and so on. Many famous math-
ematicians 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.[110]

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.

45. **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.

46. **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 [242] 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.

47. **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. 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 and http://emsh.calarts.edu/~mathart/portfolio/SPD_Costa_portfolio.html.

48. **Euler, Goldbach and the birth of ζ.** What follows is a direct transcription of correspondence between Euler and Goldbach [178], leading to the origin of the zeta function and multi-zeta values.

(a) **59. Goldbach an Euler, Moskau, 24. Dez. 1742** [footnote: AAL: F.136, Op. 2, Nr.8, Blatt 54–55]

[. . .] Als ich neulich die vermeinten summas der beiden letzteren 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[1].

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

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

$$/54r/1 + \frac{1}{2^n}\left(1 + \frac{1}{2^m}\right) + \frac{1}{3^n}\left(1 + \frac{1}{2^m} + \frac{1}{3^m}\right)$$
$$+ \frac{1}{4^n}\left(1 + \frac{1}{2^m} + \frac{1}{3^m} + \frac{1}{4^m}\right) + etc.$$

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

$$1 + \frac{1}{2^3}\left(1 + \frac{1}{2}\right) + \frac{1}{3^3}\left(1 + \frac{1}{2} + \frac{1}{3}\right) + \frac{1}{4^3}\left(1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4}\right) + etc. = \frac{\pi^4}{72}.$$

(wenn π gewöhnlichermaßen für die peripheriam circuli, cuius diameter $= 1$, genommen wird), hingegen wieß ich die summas serierum

$$A \cdots 1 + \frac{1}{2^5}\left(1 + \frac{1}{2}\right) + \frac{1}{3^5}\left(1 + \frac{1}{2} + \frac{1}{3}\right) + \frac{1}{4^5}\left(1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4}\right) + etc.$$

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

noch nicht, ob ich gleich weiß, daß $2A + B = \frac{19\pi^6}{2\cdot5\cdot7\cdot3^4}$, wie ich denn auch die summam der folgenden beiden /55/ serieum $C+D$ allezeit finden kann, si m et n sint numeri pares quicunque

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

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

---

[1]Frei zitiert nach Marcus Valerius Martialis, I, 21,9

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

(b) *"Lisez Euler, lisez Euler, c'est notre maitre a tous."* [131]

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 sen-
tence above translates as follows:

> When I recently considered further the indicated sums of
> the last two series in my previous letter, I realized immedi-
> ately 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 mi-
> nus*). [Translation thanks to Martin Matmüller, scientific
> collaborator of Euler's *Opera Omnia*, vol. IVA4, Birkhuser
> 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).

49. **Gauss: the next generation.**

> 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 [206])

50. **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)

51. **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* [253, pg. 238–9])
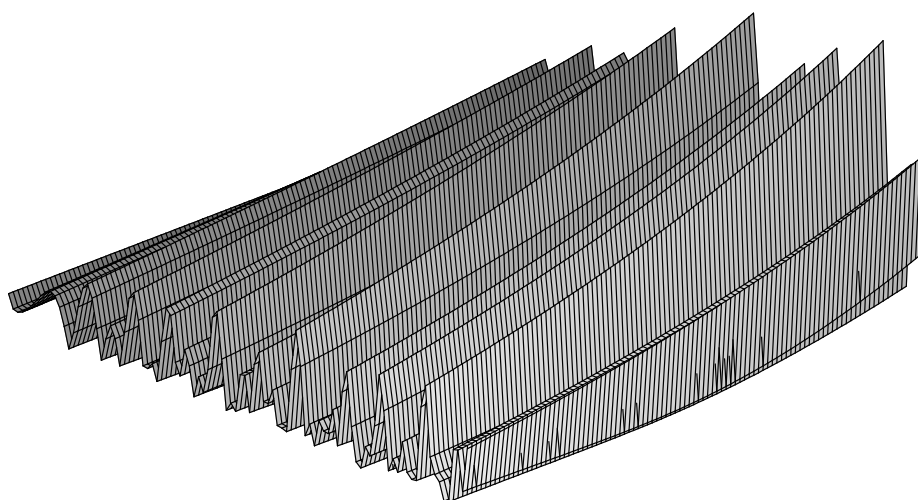
Figure 2.20. The modulus of the zeta function.

3 | Pi and Its Friends

> I am ashamed to tell you to how many figures I carried these computations, 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 π, the ratio of the circumference of a circle to its diameter, has challenged mathematicians for many centuries. In recent years, π computations have provided some fascinating examples of computational mathematics. But first, a little historical background, which we have condensed from a 1997 article [23]. Additional historical details are available from the fascinating new book *Pi Unleashed* [10], and from [74, 49]. 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. This is particularly good for biographical information about historical mathematicians, including those involved with π.

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 π 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 π, 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

$$
\begin{aligned}
a_{n+1} &= \frac{2a_n b_n}{a_n + b_n} \\
b_{n+1} &= \sqrt{a_{n+1} b_n}.
\end{aligned}
\tag{3.1}
$$

This recursion converges to π, 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 π for the next 1,800 years. For example, the Chinese mathematician Tsu Chung-Chih used a variation of this method to compute π 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 π 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 [173]. 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. [173, pg. 577]

In the 17th century, Newton and Leibniz discovered calculus, and this powerful new tool was quickly exploited to find new formulas for π. One

early calculus-based formula comes from the integral

$$\arctan x = \int_0^x \frac{dt}{1+t^2} = \int_0^x (1 - t^2 + t^4 - t^6 + \cdots)\, dt$$

$$= x - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} + \frac{x^9}{9} - \cdots . \tag{3.2}$$

Substituting $x = 1$ gives the well-known Gregory–Leibniz formula

$$\pi/4 = 1 - 1/3 + 1/5 - 1/7 + 1/9 - 1/11 + \cdots \tag{3.3}$$

(recall our discussion of Gregory's series in Section 2.2). This particular series is practically useless for computing π—it converges so slowly that hundreds of terms would be required to compute even two correct digits. However, by employing a trigonometric identity

$$\pi/4 = \arctan(1/2) + \arctan(1/3), \tag{3.4}$$

attributed to Euler in 1738, you can obtain

$$\pi/4 = \frac{1}{2} - \frac{1}{3 \cdot 2^3} + \frac{1}{5 \cdot 2^5} - \frac{1}{7 \cdot 2^7} + \cdots$$
$$+ \frac{1}{3} - \frac{1}{3 \cdot 3^3} + \frac{1}{5 \cdot 3^5} - \frac{1}{7 \cdot 3^7} + \cdots , \tag{3.5}$$

which converges much more rapidly. An even faster formula, discovered a generation earlier by Machin, can be obtained using the identity

$$\pi/4 = 4\arctan(1/5) - \arctan(1/239) \tag{3.6}$$

in a similar way. This formula was used in numerous computations of π, culminating with Shanks' computation of π 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

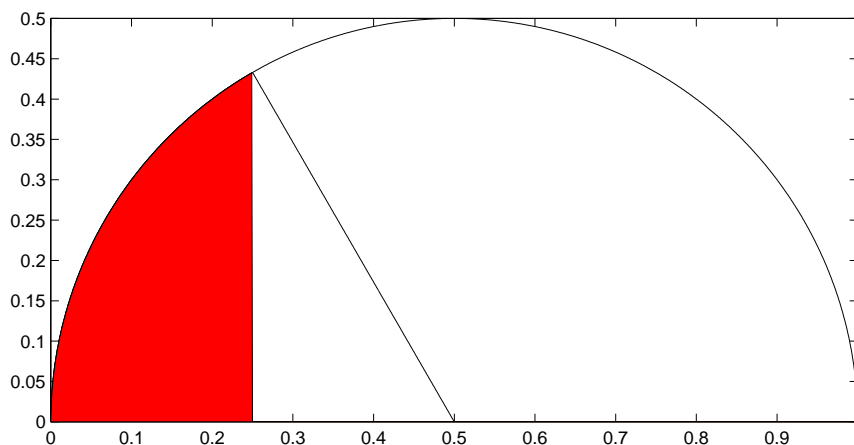$$A = \int_0^{1/4} \sqrt{x - x^2}\, dx. \tag{3.7}$$

Figure 3.1. Newton's scheme to compute π.

By employing his own binomial theorem, Newton wrote (3.7) as:

$$
\begin{aligned}
A &= \int_0^{1/4} x^{1/2}(1-x)^{1/2}\, dx \\
&= \int_0^{1/4} x^{1/2}\left(1 - x/2 - x^2/8 - x^3/16 - 5x^4/128 - \cdots\right)\, dx \\
&= \int_0^{1/4}\left(x^{1/2} - \frac{x^{3/2}}{2} - \frac{x^{5/2}}{8} - \frac{x^{7/2}}{16} - \frac{5x^{9/2}}{128} - \cdots\right)\, dx. \quad (3.8)
\end{aligned}
$$

Integrating this series term-by-term and combining the above results yielded the formula

$$
\pi = \frac{3\sqrt{3}}{4} + 24\left(\frac{1}{3\cdot 8} - \frac{1}{5\cdot 32} - \frac{1}{7\cdot 128} - \frac{1}{9\cdot 512} - \cdots\right). \quad (3.9)
$$

Newton personally used this formula to compute π. 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 π 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

$$\pi/4 \;=\; \arctan(1/2) + \arctan(1/5) + \arctan(1/8), \qquad (3.10)$$

he calculated π 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 π that until recently was not well known. For example, the Chinese mathematician Tsu Chung-Chih used a variation of Archimedes' method to compute π correct to seven digits in the fifth century. A millennium later Al-Kāshi in Samarkand, "who could calculate as eagles can fly," computed 2π 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 π (3.3) at least 200 years before Gregory or Leibniz found it. He also derived the variant series

$$\pi \;=\; \sqrt{12}\left(1 - \frac{1}{3\cdot 3} + \frac{1}{5\cdot 3^2} - \frac{1}{7\cdot 3^3} + \cdots\right), \qquad (3.11)$$

and used it to compute π to 11 decimal places. For additional information, see [49] and the MacTutor web site.

One motivation for computations of π was very much in the spirit of modern experimental mathematics: to see if the decimal expansion of π repeats, which would mean that π is the ratio of two integers (i.e., rational), or to recognize π as some algebraic constant. The question of the rationality of π was settled in the late 1700s, when Lambert and Legendre proved that the constant is irrational. The question of whether π 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 π.

In 1945, Ferguson utilized some mechanical calculating machines to compute π to 530 decimal digits, using the formula

$$\frac{\pi}{4} \ = \ 3\arctan\left(\frac{1}{4}\right) + \arctan\left(\frac{1}{20}\right) + \arctan\left(\frac{1}{1985}\right), \quad (3.12)$$

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 π was performed in 1949 on the original ENIAC. This calculation was suggested by John von Neumann, who wished to study the digits of π and e. Computing 2037 decimal places of π 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 π and other mathematical constants to high precision. These techniques will be discussed more in Section 6.2. See also [13] and [86].

In spite of these advances, until the 1970s all computer evaluations of π 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 [161, 75, 51]. One of these series is the remarkable formula

$$\frac{1}{\pi} \ = \ \frac{2\sqrt{2}}{9801}\sum_{k=0}^{\infty}\frac{(4k)!(1103+26390k)}{(k!)^4 396^{4k}}. \quad (3.13)$$

Each term of this series produces an additional *eight* correct digits in the result. Gosper used this formula to compute 17 million digits of π in 1985. Gosper also computed the first 17 million terms of the continued fraction expansion of π. 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.
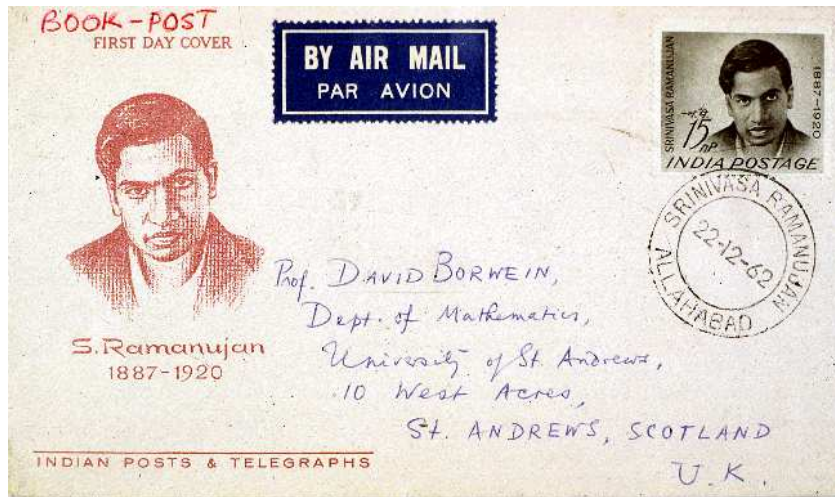
Figure 3.2. Ramanujan's 75th birthday stamp. Courtesy of Naomi Borwein.

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

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

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 π, culminating with a computation to over four billion decimal digits in 1994.

Along this line, it is interesting to note that the Ramanujan-type series (see [74, pg. 188]

$$\frac{1}{\pi} \;=\; \sum_{n=0}^{\infty} \left(\frac{\binom{2n}{n}}{16^n} \right)^3 \frac{42\,n + 5}{16} \qquad (3.15)$$

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 π 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 π 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 π). The Salamin–Brent algorithm may be stated as follows. Set $a_0 = 1, b_0 = 1/\sqrt{2}$ and $s_0 = 1/2$. Calculate

$$
\begin{aligned}
a_k &= \frac{a_{k-1} + b_{k-1}}{2} \\
b_k &= \sqrt{a_{k-1} b_{k-1}} \\
c_k &= a_k^2 - b_k^2 \\
s_k &= s_{k-1} - 2^k c_k \\
p_k &= \frac{2a_k^2}{s_k}.
\end{aligned}
\tag{3.16}
$$

Then p_k converges *quadratically* to π: 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 π. Twenty-five iterations are sufficient to compute π 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 [74]. One is as follows. Set $a_0 = 1/3$ and $s_0 = (\sqrt{3} - 1)/2$. Iterate

$$
\begin{aligned}
r_{k+1} &= \frac{3}{1 + 2(1 - s_k^3)^{1/3}} \\
s_{k+1} &= \frac{r_{k+1} - 1}{2} \\
a_{k+1} &= r_{k+1}^2 a_k - 3^k(r_{k+1}^2 - 1).
\end{aligned}
\tag{3.17}
$$

Then $1/a_k$ converges *cubically* to π—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

$$
\begin{aligned}
y_{k+1} &= \frac{1 - (1 - y_k^4)^{1/4}}{1 + (1 - y_k^4)^{1/4}} \\
a_{k+1} &= a_k(1 + y_{k+1})^4 - 2^{2k+3} y_{k+1}(1 + y_{k+1} + y_{k+1}^2).
\end{aligned}
\tag{3.18}
$$

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 π over the past 15 years or so, including his 1999 computation of π to more than 206 billion decimal digits.

Daniel Shanks, who in 1961 computed π 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 π [169]. 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 π [229, 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 π. 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 π 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 the first edition of 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 π to over 1.24 *trillion* decimal digits. Kanada and his team first computed π in hexadecimal (base 16) to 1,030,700,000,000 places, using the following two arctangent relations for π:

$$
\begin{aligned}
\pi &= 48\arctan\frac{1}{49} + 128\arctan\frac{1}{57} - 20\arctan\frac{1}{239} + 48\arctan\frac{1}{110443}\\
\pi &= 176\arctan\frac{1}{57} + 28\arctan\frac{1}{239} - 48\arctan\frac{1}{682} + 96\arctan\frac{1}{12943}.
\end{aligned}
\tag{3.19}
$$

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 Tbyte (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, `B4466E8D21 5388C4E014`, perfectly agreed with the corresponding digits produced by the two arctan formulas. At this point they converted their hexadecimal value of π 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 [181].

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 π, 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.super-computing.org. Additional historical background on record-breaking computations of π is available at http://www.cecm.sfu.ca/personal/jborwein/pi_cover.html. A listing of some milestones in the history of the computation of π is given in Tables 3.1, 3.2, and 3.3.

In retrospect, one might wonder why in antiquity π was not measured to an accuracy in excess of 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)

Name	Year	Digits	Value
Babylonians	2000? BCE	1	3.125 $(3\frac{1}{8})$
Egyptians	2000? BCE	1	3.16045 $(4(\frac{8}{9})^2)$
China	1200? BCE	1	3
Bible (1 Kings 7:23)	550? BCE	1	3
Archimedes	250? BCE	3	3.1418 (ave.)
Chang Hong	130 CE	1	3.1622 $(\sqrt{10})$
Ptolemy	150 CE	3	3.14166
Wang Fau	250 CE	1	3.15555 $(\frac{142}{45})$
Liu Hui	263 CE	5	3.14159
Siddhanta	380 CE	3	3.1416
Tsu Ch'ung Chi	480 CE	7	3.1415926 (355/113)
Aryabhata	499 CE	4	3.14156 (62832/2000)
Brahmagupta	640 CE	1	3.162277 $(= \sqrt{10})$
Al-Khowarizmi	800 CE	4	3.1416
Fibonacci	1220 CE	3	3.141818
Madhava	1400 CE	11	3.14159265359
Al-Kāshi	1429 CE	14	3.14159265358979
Otho	1573 CE	6	3.1415929
Viéte	1593 CE	9	3.1415926536 (ave.)
Romanus	1593 CE	15	3.141592653589793
Van Ceulen	1596 CE	20	3.14159265358979323846
Van Ceulen	1615 CE	35	

Table 3.1. Pre-calculus era π calculations.

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

Table 3.2. Calculus era π calculations.

Name	Year	Digits
Ferguson	1946	620
Ferguson	1947	710
Ferguson and Wrench	1947	808
Smith and Wrench	1949	1,120
Reitwiesner et al. (ENIAC)	1949	2,037
Nicholson and Jeenel	1954	3,092
Felton	1957	7,480
Genuys	1958	10,000
Felton	1958	10,021
Guilloud	1959	16,167
Shanks and Wrench	1961	100,265
Guilloud and Filliatre	1966	250,000
Guilloud and Dichampt	1967	500,000
Guilloud and Bouyer	1973	1,001,250
Miyoshi and Kanada	1981	2,000,036
Guilloud	1982	2,000,050
Tamura	1982	2,097,144
Tamura and Kanada	1982	4,194,288
Tamura and Kanada	1982	8,388,576
Kanada, Yoshino and Tamura	1982	16,777,206
Ushiro and Kanada	Oct. 1983	10,013,395
Gosper	Oct. 1985	17,526,200
Bailey	Jan. 1986	29,360,111
Kanada and Tamura	Sep. 1986	33,554,414
Kanada and Tamura	Oct. 1986	67,108,839
Kanada, Tamura, Kubo, et. al	Jan. 1987	134,217,700
Kanada and Tamura	Jan. 1988	201,326,551
Chudnovskys	May 1989	480,000,000
Chudnovskys	Jun. 1989	525,229,270
Kanada and Tamura	Jul. 1989	536,870,898
Kanada and Tamura	Nov. 1989	1,073,741,799
Chudnovskys	Aug. 1989	1,011,196,691
Chudnovskys	Aug. 1991	2,260,000,000
Chudnovskys	May 1994	4,044,000,000
Takahashi and Kanada	Jun. 1995	3,221,225,466
Kanada	Aug. 1995	4,294,967,286
Kanada	Oct. 1995	6,442,450,938
Kanada and Takahashi	Jun. 1997	51,539,600,000
Kanada and Takahashi	Sep. 1999	206,158,430,000
Kanada, Ushiro, Kuroda, Kudoh	Dec. 2002	1,241,100,000,000

Table 3.3. Digital era π calculations.

> 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 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 π. Kanada, for example, has performed detailed statistical analysis of his computed results of π to see if there are any statistical abnormalities that suggest π 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 π 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 π (see, for example, http://www.piworld.de), and thousands of online research papers and other documents dealing with π. There are even several Internet-based clubs devoted to π, one of which requires that initiates recite by heart the first 100 digits of π with "respect, fluency, and smoothness" (see http://pi314.at). The very popular web-site http://www.cecm.sfu.ca/pi/yapPing.html recites π in many different languages.

Fascination with π is also evident in the many recent popular books, television shows, and movies that have mentioned π. In the 1967 *Star Trek* episode "Wolf in the Fold," Spock foiled the evil computer by telling it to compute the last digit of π. A May 1993 segment of *The Simpsons* featured the character Apu boasting that he can recite π 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) [221]. In November 1996, the MSNBC network aired a news segment about π, 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 π, and after her mysterious experience found confirmation in the base-11 expansion of π [251]. A 1997 book entitled *The Joy of Pi* sold thousands of copies [54]. A 1998 movie entitled *Pi* began with decimal digits of π displayed on the screen. The 2001 Academy Award-winning movie *A Beautiful Mind*, which portrayed the life of mathematician John Nash, shows π in equations scribbled by the lead actor Russell Crowe (although the π 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 [214]. 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 π [115].

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 π.

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

$$\alpha(N) = \frac{E'(k_N)}{K(k_N)} - \frac{\pi}{4\,K^2(k_N)} \tag{3.20}$$

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):

$$
\begin{aligned}
\alpha(1) &\approx 0.49999999999999999999 \\
\alpha(2) &\approx 0.41421356237309504880 \\
\alpha(3) &\approx 0.36602540378443864678 \\
\alpha(5) &\approx 0.33188261099247156221 \\
\alpha(7) &\approx 0.32287565553229529536.
\end{aligned}
$$

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

$$\alpha(5) \quad = \quad \frac{\sqrt{5} - \sqrt{2\sqrt{5}-2}}{2}. \tag{3.21}$$

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 π: let $\alpha_0 = \alpha(N)$ and $k_0 = k'_N$ (where $k' = \sqrt{1-k^2}$) and iterate

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

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

Then

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

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 π. On closer inspection while the provable cases were correct to $5,000$ digits, the empirical ones agreed with π to roughly 100 places only. Now, in many ways to have discovered a "natural" number that agreed with π 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 π has been discovered. For example, this sentiment is suggested in the closing chapters of Beckmann's 1971 book on the history of π [48, 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 π, which permits successive digits of π (in any desired base) to be computed with a relatively simple recursive algorithm based on the previously generated digits (see [238] 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 π, 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 π. In 1996, Peter Borwein, Simon Plouffe, and one of the present authors (Bailey) found an algorithm for computing individual hexadecimal or binary digits of π [33]. To be precise, this algorithm:

(1) directly produces a modest-length string of digits in the hexadecimal or binary expansion of π, 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 π 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 π 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 π:

Theorem 3.2.

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

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

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

$$=\; \frac{1}{2^{k/2}} \sum_{i=0}^{\infty} \frac{1}{16^i(8i+k)}. \qquad (3.26)$$

Thus one can write

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

$$=\; \int_0^{1/\sqrt{2}} \frac{4\sqrt{2} - 8x^3 - 4\sqrt{2}x^4 - 8x^5}{1-x^8}\, dx, \qquad (3.27)$$

which on substituting $y = \sqrt{2}x$ becomes

$$\int_0^1 \frac{16\, y - 16}{y^4 - 2\, y^3 + 4\, y - 4}\, dy \;=\; \int_0^1 \frac{4y}{y^2 - 2}\, dy - \int_0^1 \frac{4y - 8}{y^2 - 2y + 2}\, dy$$

$$=\; \pi. \qquad (3.28)$$

$\square$

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 $\log 2$:

$$\log 2 \;=\; \sum_{k=0}^{\infty} \frac{1}{k2^k}. \qquad (3.29)$$

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

$$
\begin{aligned}
\{2^d \log 2\} &= \left\{ \left\{ \sum_{k=0}^{d} \frac{2^{d-k}}{k} \right\} + \sum_{k=d+1}^{\infty} \frac{2^{d-k}}{k} \right\} \\
&= \left\{ \left\{ \sum_{k=0}^{d} \frac{2^{d-k} \bmod k}{k} \right\} + \sum_{k=d+1}^{\infty} \frac{2^{d-k}}{k} \right\}. \qquad (3.30)
\end{aligned}
$$

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 $2^{d-k} \bmod k$, 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 [187, 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 $r = b^n \bmod k$, 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: if $n \geq t$ then $r \leftarrow br \bmod k$; $\quad n \leftarrow n - t$; $\quad$ endif
> $t \leftarrow t/2$
> if $t \geq 1$ then $r \leftarrow r^2 \bmod k$; $\quad$ go to A; $\quad$ endif $\qquad \square$

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 $d+1$.   □

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 α of the form

$$\alpha \;=\; \sum_{k=0}^{\infty} \frac{p(k)}{q(k)2^k}, \tag{3.31}$$

where $p(k)$ and $q(k)$ are integer polynomials, with $\deg p < \deg q$ 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 π also shares this property did not escape these researchers. Unfortunately, exhaustive searches of the mathematical literature did not uncover any formula for π 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 π. 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 [139, 16]. 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 $\sum_i a_i \alpha_i = 0$, to within a very small "epsilon." After a month or two of computation, with numerous restarts using new α vectors (when additional formulas were found in the literature) the identity (3.25) was finally uncovered. The actual formula found by the computation was:

$$\pi \quad = \quad 4F(1/4, 5/4; 1; -1/4) + 2\arctan(1/2) - \log 5, \qquad (3.32)$$

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

$$\pi \quad = \quad \sum_{i=0}^{\infty} \frac{1}{16^i}\left(\frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6}\right). \qquad (3.33)$$

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

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

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

$$\{16^d\pi\} \quad = \quad \{4\{16^d S_1\} - 2\{16^d S_4\} - \{16^d S_5\} - \{16^d S_6\}\}, \quad (3.35)$$

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

$$\{16^d S_j\} = \left\{ \left\{ \sum_{k=0}^{d} \frac{16^{d-k}}{8k+j} \right\} + \sum_{k=d+1}^{\infty} \frac{16^{d-k}}{8k+j} \right\}$$

$$= \left\{ \left\{ \sum_{k=0}^{d} \frac{16^{d-k} \bmod 8k+j}{8k+j} \right\} + \sum_{k=d+1}^{\infty} \frac{16^{d-k}}{8k+j} \right\} \quad (3.36)$$

instead of Equation (3.30), to compute $\{16^d S_j\}$ 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. $\square$

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 [33]. 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 discovered 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 researchers. 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).

Position	Hex Digits Beginning at This Position
10^6	26C65E52CB4593
10^7	17AF5863EFED8D
10^8	ECB840E21926EC
10^9	85895585A0428B
10^{10}	921C73C6838FB2
10^{11}	9C381872D27596
1.25×10^{12}	07E45733CC790B
2.5×10^{14}	E6216B069CB6C1

Table 3.4. Computed hexadecimal digits of π.

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 computational scheme to compute individual *decimal* digits of π. Searches conducted 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) [73]. However, none of this removes the possibility that there exists some completely different approach that permits rapid computation of individual decimal digits of π. Also, as we will see in the next section, there do exist formulas for certain other constants that admit individual digit calculation schemes in various nonbinary bases (including base ten).

3.5 Unpacking the BBP Formula for Pi

It is worth asking "why" the formula

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

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

$$- 2\log 2 + 2\log(2 - \sqrt{2}) + \pi + 2\log(2 + \sqrt{2}), \tag{3.39}$$

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

$$S_b \quad = \quad \sum_{k=0}^{\infty} \frac{1}{16^k(8k + b)}$$

for $1 \le b \le 8$ and the corresponding normalized integrals

$$I(b) \quad = \quad 2^{b/2} \int_0^{1/\sqrt{2}} \frac{x^{b-1}}{1 - x^8} dx. \tag{3.40}$$

Again, *Maple* provides closed forms for $I(b)$ in which the basic quanti-
ties 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:

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

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

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

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

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

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

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

$$S_8 = 8\log 2 - 2\log 5 - 2\log 3. \tag{3.41}$$

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

$$
\begin{aligned}
\mathrm{Im}\left(\log\left(1 - \frac{1-i}{x}\right)\right) &= \arctan\left(\frac{1}{1-x}\right) \\
2\arctan(1/3) + \arctan(1/7) &= \arctan(1/2) + \arctan(1/3) \\
&= \arctan 1 \ = \ \pi/4 \qquad (3.42)
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{\pi}{4} \ = \ & \frac{1}{16}\sum_{n=0}^{\infty}\frac{(-1)^n}{64^n}\left(\frac{8}{4n+1} + \frac{4}{4n+2} + \frac{1}{4n+3}\right) \\
+ \ & \frac{1}{256}\sum_{n=0}^{\infty}\frac{(-1)^n}{1024^n}\left(\frac{32}{4n+1} + \frac{8}{4n+2} + \frac{1}{4n+3}\right), \qquad (3.43)
\end{aligned}
$$

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

$$
\alpha \ = \ \sum_{k=0}^{\infty}\frac{p(k)}{b^k q(k)}, \qquad (3.44)
$$

is now referred to as a BBP-type formula, named after the initials of the authors of the 1997 paper where the π hex digit algorithm appeared [33]. For a constant α 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 [33] 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 approach, using PSLQ searches. Others were found as the result of educated guesses based on experimentally obtained results. In each case, these formulas 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 π 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 3.5. Some nonbinary BBP-type formulas are shown in Table 3.6. These formulas are derived from several sources: [33, 93, 94]. An updated collection is available at [19]. The constant G that appears in Table 3.5 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 3.5 and 3.6, 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:

$$
\begin{aligned}
\log 3 &= 2\log 2 + \log\left(1 - \frac{1}{4}\right) = 2\sum_{k=1}^{\infty}\frac{1}{k2^k} - \sum_{k=1}^{\infty}\frac{1}{k4^k} \\
&= \frac{1}{2}\sum_{k=0}^{\infty}\frac{1}{4^k}\left(\frac{2}{2k+1} + \frac{1}{2k+2}\right) - \frac{1}{4}\sum_{k=0}^{\infty}\frac{1}{4^k}\left(\frac{2}{2k+2}\right) \\
&= \sum_{k=0}^{\infty}\frac{1}{4^k}\left(\frac{1}{2k+1}\right). \tag{3.46}
\end{aligned}
$$

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

$$
\alpha = \log\left(1 \pm \frac{(1+i)^k}{2^n}\right) \tag{3.47}
$$

yields a BBP-type formula. See [19] for details.

The logarithms of the following primes are now known to possess binary

BBP formulas [103]:

2, 3, 5, 7, 11, 13, 17, 19, 29, 31, 37, 41, 43, 61, 73, 109, 113, 127, 151,
241, 257, 331, 337, 397, 683, 1321, 1429, 1613, 2113, 2731, 5419, 8191,
14449, 26317, 38737, 43691, 61681, 65537, 87211, 131071, 174763,
246241, 262657, 268501, 279073, 312709, 524287, 525313, 599479,
2796203, 4327489, 7416361, 15790321, 18837001, 22366891   (3.48)

$$\pi\sqrt{3} = \frac{9}{32}\sum_{k=0}^{\infty}\frac{1}{64^k}\left(\frac{16}{6k+1}+\frac{8}{6k+2}-\frac{2}{6k+4}-\frac{1}{6k+5}\right)$$

$$\pi^2 = \frac{9}{8}\sum_{k=0}^{\infty}\frac{1}{64^k}\left(\frac{16}{(6k+1)^2}-\frac{24}{(6k+2)^2}-\frac{8}{(6k+3)^2}-\frac{6}{(6k+4)^2}\right.$$
$$\left.+\frac{1}{(6k+5)^2}\right)$$

$$\log^2 2 = \frac{1}{32}\sum_{k=0}^{\infty}\frac{1}{64^k}\left(\frac{64}{(6k+1)^2}-\frac{160}{(6k+2)^2}-\frac{56}{(6k+3)^2}-\frac{40}{(6k+4)^2}\right.$$
$$\left.+\frac{4}{(6k+5)^2}-\frac{1}{(6k+6)^2}\right)$$

$$\pi\log 2 = \frac{1}{256}\sum_{k=0}^{\infty}\frac{1}{4096^k}\left(\frac{4096}{(24k+1)^2}-\frac{8192}{(24k+2)^2}-\frac{26112}{(24k+3)^2}+\frac{15360}{(24k+4)^2}\right.$$
$$-\frac{1024}{(24k+5)^2}+\frac{9984}{(24k+6)^2}+\frac{11520}{(24k+8)^2}+\frac{2368}{(24k+9)^2}-\frac{512}{(24k+10)^2}$$
$$+\frac{768}{(24k+12)^2}-\frac{64}{(24k+13)^2}+\frac{408}{(24k+15)^2}+\frac{720}{(24k+16)^2}$$
$$\left.+\frac{16}{(24k+17)^2}+\frac{196}{(24k+18)^2}+\frac{60}{(24k+20)^2}-\frac{37}{(24k+21)^2}\right)$$

$$G = \frac{1}{1024}\sum_{k=0}^{\infty}\frac{1}{4096^k}\left(\frac{3072}{(24k+1)^2}-\frac{3072}{(24k+2)^2}-\frac{23040}{(24k+3)^2}+\frac{12288}{(24k+4)^2}\right.$$
$$-\frac{768}{(24k+5)^2}+\frac{9216}{(24k+6)^2}+\frac{10368}{(24k+8)^2}+\frac{2496}{(24k+9)^2}-\frac{192}{(24k+10)^2}$$
$$+\frac{768}{(24k+12)^2}-\frac{48}{(24k+13)^2}+\frac{360}{(24k+15)^2}+\frac{648}{(24k+16)^2}$$
$$\left.+\frac{12}{(24k+17)^2}+\frac{168}{(24k+18)^2}+\frac{48}{(24k+20)^2}-\frac{39}{(24k+21)^2}\right)$$

Table 3.5. Binary BBP-type formulas.

$$\log 2 = \frac{2}{3} \sum_{k=0}^{\infty} \frac{1}{9^k(2k+1)}$$

$$\pi\sqrt{3} = \frac{1}{9} \sum_{k=0}^{\infty} \frac{1}{729^k} \left(\frac{81}{12k+1} - \frac{54}{12k+2} - \frac{9}{12k+4} - \frac{12}{12k+6} \right.$$
$$\left. - \frac{3}{12k+7} - \frac{2}{12k+8} - \frac{1}{12k+10} \right)$$

$$\log 3 = \frac{1}{729} \sum_{k=0}^{\infty} \frac{1}{729^k} \left(\frac{729}{6k+1} + \frac{81}{6k+2} + \frac{81}{6k+3} + \frac{9}{6k+4} \right.$$
$$\left. + \frac{9}{6k+5} + \frac{1}{6k+6} \right)$$

$$\pi^2 = \frac{2}{27} \sum_{k=0}^{\infty} \frac{1}{729^k} \left(\frac{243}{(12k+1)^2} - \frac{405}{(12k+2)^2} - \frac{81}{(12k+4)^2} \right.$$
$$- \frac{27}{(12k+5)^2} - \frac{72}{(12k+6)^2} - \frac{9}{(12k+7)^2} - \frac{9}{(12k+8)^2}$$
$$\left. - \frac{5}{(12k+10)^2} + \frac{1}{(12k+11)^2} \right)$$

$$\log\left(\frac{9}{10}\right) = \frac{-1}{10} \sum_{k=1}^{\infty} \frac{1}{k 10^k}$$

$$\log\left(\frac{1111111111}{387420489}\right) = \frac{1}{10^8} \sum_{k=0}^{\infty} \frac{1}{10^{10k}} \left(\frac{10^8}{10k+1} + \frac{10^7}{10k+2} + \frac{10^6}{10k+3} \right.$$
$$+ \frac{10^5}{10k+4} + \frac{10^4}{10k+5} + \frac{10^3}{10k+6} + \frac{10^2}{10k+7}$$
$$\left. + \frac{10}{10k+8} + \frac{1}{10k+9} \right)$$

$$\frac{25}{2} \log\left(\frac{781}{256} \left(\frac{57-5\sqrt{5}}{57+5\sqrt{5}} \right)^{\sqrt{5}} \right) = \sum_{k=0}^{\infty} \frac{1}{5^{5k}} \left(\frac{5}{5k+2} + \frac{1}{5k+3} \right) \qquad (3.45)$$

Table 3.6. Nonbinary BBP-type formulas.

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 3.6. This has been used to compute the ten billionth decimal digit of $\log(9/10)$ [33].

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 $q = |\mathrm{Im}(T)/\mathrm{Re}(T)|$ or $|\mathrm{Re}(T)/\mathrm{Im}(T)|$, where

$$T = \prod_{k=1}^{m} \left(1 \pm \frac{i}{2^{t_k}}\right)^{u_k} \left(1 \pm \frac{1+i}{2^{v_k}}\right)^{w_k} \tag{3.49}$$

for various m-long nonnegative integer vectors t, u, v, w and choices of signs as shown [74, 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 $T = 25/32 - 5i/8$, which yields $q = 4/5$. Indeed, one can obtain the formula

$$\arctan\left(\frac{4}{5}\right) = \frac{1}{2^{17}} \sum_{k=0}^{\infty} \frac{1}{2^{20k}} \left(\frac{524288}{40k+2} - \frac{393216}{40k+4} - \frac{491520}{40k+5} + \frac{163840}{40k+8}\right.$$
$$+ \frac{32768}{40k+10} - \frac{24576}{40k+12} + \frac{5120}{40k+15} + \frac{10240}{40k+16}$$
$$+ \frac{2048}{40k+18} + \frac{1024}{40k+20} + \frac{640}{40k+24} + \frac{480}{40k+25}$$
$$+ \frac{128}{40k+26} - \frac{96}{40k+28} + \frac{40}{40k+32} + \frac{8}{40k+34}$$
$$\left. - \frac{5}{40k+35} - \frac{6}{40k+36}\right). \tag{3.50}$$

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

$$\tan(r+s) = \frac{\tan r + \tan s}{1 - \tan r \tan s}, \tag{3.51}$$

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 following rational numbers. Only those rationals

with numerators < denominators ≤ 25 are listed here.

1/2, 1/3, 2/3, 1/4, 3/4, 1/5, 2/5, 3/5, 4/5, 1/6, 5/6, 1/7, 3/7,
4/7, 5/7, 6/7, 1/8, 7/8, 1/9, 2/9, 7/9, 8/9, 3/10, 1/11, 2/11,
3/11, 7/11, 8/11, 10/11, 1/12, 5/12, 1/13, 4/13, 6/13, 7/13, 9/13,
11/13, 12/13, 3/14, 5/14, 1/15, 4/15, 8/15, 1/16, 7/16, 11/16, 13/16,
15/16, 1/17, 4/17, 6/17, 7/17, 9/17, 11/17, 15/17, 16/17, 1/18, 13/18,
3/19, 4/19, 6/19, 7/19, 8/19, 9/19, 11/19, 17/19, 9/20, 1/21, 13/21,
16/21, 20/21, 3/22, 7/22, 9/22, 19/22, 21/22, 2/23, 4/23, 6/23, 7/23,
9/23, 10/23, 11/23, 14/23, 15/23, 7/24, 11/24, 23/24, 1/25, 2/25,
13/25, 19/25, 21/25   (3.52)

Note that not all "small" rationals appear in this list. As it turns out, by
applying the methods given in the paper [73] (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 (3.49), 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
(3.49).

3.7   Does Pi Have a Nonbinary BBP Formula?

As we mentioned above, from the day that the BBP-formula for π 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 π^2, as
well as for $\log 2$ (see Tables 3.5 and 3.6). But extensive computations failed
to find any nonbinary formulas for π.

   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 π. We believe that if there is no nonbinary
Machin-type arctangent formula for π, then there is no nonbinary BBP-

type formula of any form for π. We will summarize this result here. Full details and other related results can be found in [73].

We say that the integer $b > 1$ is not a proper power if it cannot be written as c^m for any integers c and $m > 1$. We will use the notation $\operatorname{ord}_p(z)$ to denote the p-adic order of the rational $z \in Q$. In particular, $\operatorname{ord}_p(p) = 1$ for prime p, while $\operatorname{ord}_p(q) = 0$ for primes $q \neq p$, and $\operatorname{ord}_p(wz) = \operatorname{ord}_p(w) + \operatorname{ord}_p(z)$. The notation $\nu_b(p)$ 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 $\nu_b(p) = m$. Given the Gaussian integer $z \in Q[i]$ and the rational prime $p \equiv 1 \pmod 4$, let $\theta_p(z)$ denote $\operatorname{ord}_{\mathfrak{p}}(z) - \operatorname{ord}_{\overline{\mathfrak{p}}}(z)$, where $\mathfrak{p}$ and $\overline{\mathfrak{p}}$ are the two conjugate Gaussian primes dividing p, and where we require $0 < \Im(\mathfrak{p}) < \mathrm{R}(\mathfrak{p})$ to make the definition of θ_p unambiguous. Note that

$$\theta_p(wz) \quad = \quad \theta_p(w) + \theta_p(z). \tag{3.53}$$

Given $\kappa \in R$, with $2 \leq b \in Z$ and b not a proper power, we say that κ has a Z-linear or Q-linear *Machin-type BBP arctangent formula* to the base b if and only if κ can be written as a Z-linear or Q-linear combination (respectively) of generators of the form

$$\arctan\left(\frac{1}{b^m}\right) \quad = \quad \Im \log\left(1 + \frac{i}{b^m}\right) \quad = \quad b^m \sum_{k=0}^{\infty} \frac{(-1)^k}{b^{2mk}(2k+1)}. \tag{3.54}$$

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 $b = 2^N - 1$, $N \in Z$, $m = 2$, $b^m - 1 = 2^{N+1}(2^{N-1} - 1)$.*

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 Q-linear Machin-type BBP arctangent formula for π.*

Proof. It follows immediately from the definition of a Q-linear Machin-type BBP arctangent formula that any such formula has the form

$$\pi \quad = \quad \frac{1}{n} \sum_{m=1}^{M} n_m \Im \log(b^m - i) \tag{3.55}$$

where $n > 0 \in Z$, $n_m \in Z$, and $M \geq 1$, $n_M \neq 0$. This implies that

$$\prod_{m=1}^{M} (b^m - i)^{n_m} \in e^{ni\pi} Q^{\times} \quad = \quad Q^{\times} \tag{3.56}$$

For any $b > 2$ and not a proper power we have $M_b \leq 2$, so 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 $p \equiv 1$ (mod 4), and that p factors as $p = \mathfrak{p}\overline{\mathfrak{p}}$ over $Z[i]$, with exactly one of $\mathfrak{p}$, $\overline{\mathfrak{p}}$ dividing $b^M - i$. Referring to the definition of θ, we see that we must have $\theta_p(b^M - i) \neq 0$. Furthermore, for any $m < M$, neither $\mathfrak{p}$ nor $\overline{\mathfrak{p}}$ can divide $b^m - i$ since this would imply $p \mid b^{4m} - 1$, $4m < 4M$, 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 (3.55), using Equation (3.53) and the fact that $n_M \neq 0$, we get the contradiction

$$0 \quad \neq \quad n_M \theta_p(b^M - i) \ = \ \sum_{m=1}^{M} n_m \theta_p(b^m - i) \ = \ \theta_p(Q^{\times}) = 0. \tag{3.57}$$

Thus our assumption that there was a b-ary Machin-type BBP arctangent formula for π must be false. $\square$

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

Figure 3.3. The ENIAC computer. Courtesy of Smithsonian Institution.

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 π:

$$\pi \approx \frac{3}{\sqrt{163}} \, \log{(640320)},$$

correct to 15 decimal places, and

$$\pi \approx \frac{3}{\sqrt{67}} \, \log{(5280)},$$

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 π approximations:

$$\pi \approx 66 \, \frac{\sqrt{2}}{33\,\sqrt{29} - 148}$$

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

$$\begin{aligned}
\pi \;=\;\; & a_1 \arctan \frac{1}{390112} + a_2 \arctan \frac{1}{485298} \\
& + a_3 \arctan \frac{1}{683982} + a_4 \arctan \frac{1}{1984933} \\
& + a_5 \arctan \frac{1}{2478328} + a_6 \arctan \frac{1}{3449051} \\
& + a_7 \arctan \frac{1}{18975991} + a_8 \arctan \frac{1}{22709274} \\
& + a_9 \arctan \frac{1}{24208144} + a_{10} \arctan \frac{1}{201229582} \\
& + a_{11} \arctan \frac{1}{2189376182}
\end{aligned}$$

holds [10, 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://oldweb.cecm.sfu.ca/projects/IntegerRelations or http://www.experimentalmath.info.

4. **Ballantine's series for pi.** A formula of Euler for arccot is

$$x \sum_{n=0}^{\infty} \frac{(n!)^2 \, 4^n}{(2\,n+1)! \, (x^2+1)^{n+1}} \;=\; \arctan\left(\frac{1}{x}\right). \qquad (3.58)$$

As observed by Ballantine in 1939, ([49]) this allows one to rewrite the variant of Machin's formula, used by Guilloud and Bouyer in 1973 to compute a million digits of π,

$$\frac{\pi}{4} \;=\; 12 \arctan \frac{1}{18} + 8 \arctan \frac{1}{57} - 5 \arctan \frac{1}{239} \qquad (3.59)$$

in the neat form

$$\begin{aligned}
\pi \;=\;\; & 864 \sum_{n=0}^{\infty} \frac{(n!)^2 \, 4^n}{(2\,n+1)! \, 325^{n+1}} + 1824 \sum_{n=0}^{\infty} \frac{(n!)^2 \, 4^n}{(2\,n+1)! \, 3250^{n+1}} \\
& - 20 \arctan \frac{1}{239}, \qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.60)
\end{aligned}$$

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 [48, 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." [212]

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^π, which can be computed using the following iteration.

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

   Set $k_0 = 1/\sqrt{2}$ and for $n < N = \lceil \log_2(D/1.36) \rceil$ iterate

   $$k'_n = \sqrt{1 - k_n^2}, \qquad k_{n+1} = \frac{1 - k'_n}{1 + k'_n}.$$

   Then return

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

   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 Γ 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

   $$x_{n+1} = \frac{\sqrt{x_n} + 1/\sqrt{x_n}}{2} \tag{3.61}$$

   $$y_{n+1} = \frac{y_n \sqrt{x_n} + 1/\sqrt{x_n}}{y_n + 1}. \tag{3.62}$$

   Then

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

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

   No such iteration is known for $\Gamma\left(\frac{1}{5}\right)$; see [74, 68].

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*

$$\gamma = \lim_{n\to\infty} \sum_{k=1}^{n} \frac{1}{k} - \log(n) \tag{3.63}$$

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 ([74, pg. 336]), is based on Bessel function identities. It allows one to show that if γ is rational it must have a denominator with millions of digits. The underlying identity, known to Euler, is

$$\gamma + \log(z/2) = \frac{S_0(z) - K_0(z)}{I_0(z)} \tag{3.64}$$

where $I_\nu(z) = \sum_{k=0}^\infty (z/2)^{2k+\nu}/(k!\,\Gamma(k + \nu + 1))$, while $K_0(z) = \partial I_0(z)/\partial\nu$ and $S_0(z) = \sum_{k=0}^\infty (\sum_{j=1}^k 1/j)\,(z/2)^{2k}/(k!)^2$.

An algorithm follows from knowing the first terms of the asymptotic expansion for K_0 and I_0. It is

Algorithm 3.10. *Computation of K_0 and I_0:*

$A_0 = -\log(n), B_0 = 1, U_0 = A_0, V_0 = 1$, and for $k = 1, 2, \cdots$,

$$\begin{aligned}
B_k &= B_{k-1}n^2/k^2, & A_k &= (A_{k-1}n^2/k + B_k)/k, \\
U_k &= U_{k-1} + A_k, & V_k &= V_{k-1} + B_k.
\end{aligned} \tag{3.65}$$

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 γ 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 π (millions of trials would be required to obtain just a few digits), it is an instructive example of how π 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.

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 π appearing in a number-theory setting. See [162].

14. **The irrationality of pi.** We reproduce in extenso Ivan Niven's 1947 very concise proof that π is irrational [223].

    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

    $$\int_0^\pi f(x)\sin x\,dx = [F'(x)\sin x - F(x)\cos x]_0^\pi = F(\pi) + F(0). \quad (3.66)$$

    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 (3.66) is *positive but arbitrarily small* for n sufficiently large. Thus (3.66) is false, and so is our assumption that π is rational. □

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") [238]. 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 $e = \sum 1/i!$.

$$e \;=\; 1 + \frac{1}{1}\left(1 + \frac{1}{2}\left(1 + \frac{1}{3}\left(1 + \frac{1}{4}\left(1 + \frac{1}{5}\left(1 + \cdots\right)\right)\right)\right)\right).$$

   (b) Implement a parallel spigot algorithm for π, 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 π "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 π 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 π, which is a poor method to compute π, 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 π, 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 $x_n = cx_{n-1} \bmod 2^{32}$, where $c = 5^9 = 1953125$. This generator is of the well known class of linear congruential generators and has period 2^{30} [187, 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^{53}. 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 π, 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. *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 $(x_{km}, x_{km+1}, x_{km+2}, \cdots, x_{km+m-1})$. Note that the starting value x_{km} for processor k can be directly computed as $x_{km} = 5^{9km}x_0 \bmod 2^{32}$. 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. **Life of Pi.** At the end of his story, Piscine (Pi) Molitor [214, 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 π to be irrational.

4 | Normality of Numbers

> Anyone who wants to make a name for himself can examine the major issue of whether π is *normal*, or perhaps more accurately, whether π 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 α and an integer $b > 2$, we say that α is *b-normal* or *normal base b* if *every* sequence of k consecutive digits in the base-b expansion of α 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 α 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

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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 π, 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 [99, 141]. In addition to the widely recognized constants such as π and e, we have listed Catalan's constant (G), Euler's constant (γ), 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 α and δ constants, Khintchine's constant $\mathcal{K}$, and Madelung's constant $\mathcal{M}_3$. Binary values for some of these constants, as well as Chaitin's Ω constant (from the field of computational complexity) [99], are given in Table 4.2. As you can see, none of the expansions in either table exhibits any evident "pattern."

The digits of π have been studied more than any other single constant, in part because of the widespread fascination with π. 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 π. These counts are shown in Table 4.3. For reasons given in Section 3.4, binary (or hexadecimal) digits of π 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. 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 π. Along this line, a graphic based on a random walk of the first million decimal digits of π, 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 π, 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

Constant	Value
$\sqrt{2}$	$1.4142135623730950488\ldots$
$\sqrt{3}$	$1.7320508075688772935\ldots$
$\sqrt{5}$	$2.2360679774997896964\ldots$
$\phi = \frac{\sqrt{5}-1}{2}$	$0.61803398874989484820\ldots$
π	$3.1415926535897932384\ldots$
$1/\pi$	$0.31830988618379067153\ldots$
e	$2.7182818284590452353\ldots$
$1/e$	$0.36787944117144232159\ldots$
e^π	$23.140692632779269005\ldots$
$\log 2$	$0.69314718055994530941\ldots$
$\log 10$	$2.3025850929940456840\ldots$
$\log_2 10$	$3.3219280948873623478\ldots$
$\log_{10} 2$	$0.30102999566398119522\ldots$
$\log_2 3$	$1.5849625007211561814\ldots$
$\zeta(2)$	$1.6449340668482264364\ldots$
$\zeta(3)$	$1.2020569031595942854\ldots$
$\zeta(5)$	$1.0369277551433699263\ldots$
G	$0.91596559417721901505\ldots$
γ	$0.57721566490153286060\ldots$
$\Gamma(1/2) = \sqrt{\pi}$	$1.7724538509055160272\ldots$
$\Gamma(1/3)$	$2.6789385347077476336\ldots$
$\Gamma(1/4)$	$3.6256099082219083119\ldots$
$K(1/\sqrt{2})$	$1.8540746773013719184\ldots$
$E(1/\sqrt{2})$	$1.3506438810476755025\ldots$
α_f	$4.6692016091029906718\ldots$
δ_f	$2.5029078750958928222\ldots$
$\mathcal{K}$	$2.6854520010653064453\ldots$
$\mathcal{M}_3$	$1.7475645946331821903\ldots$

Table 4.1. Decimal values of various mathematical constants.

Constant	Value
π	$11.00100100001111110110101010001000100001011010001100001001\ldots$
e	$10.10110111111000010101000101100010100010101011101101001010100\ldots$
$\sqrt{2}$	$1.0110101000001001111001100110011111111001110111100110010010\ldots$
$\sqrt{3}$	$1.1011101101100111101011101000010110000100110010101010011100\ldots$
$\log 2$	$0.1011000101110010000101111111101111101000111001111011110011\ldots$
$\log 3$	$1.0001100100111110101001110101010101101000000110000101010101\ldots$
Ω	$0.0000001000000100001000001000011101110011001001111000100100\ldots$

Table 4.2. Binary values of various mathematical constants.

Digit	Occurrences
0	99999485134
1	99999945664
2	100000480057
3	99999787805
4	100000357857
5	99999671008
6	99999807503
7	99999818723
8	100000791469
9	99999854780
Total	1000000000000

Table 4.3. Statistics for the first trillion decimal digits of π.

Digit	Occurrences
0	62499881108
1	62500212206
2	62499924780
3	62500188844
4	62499807368
5	62500007205
6	62499925426
7	62499878794
8	62500216752
9	62500120671
A	62500266095
B	62499955595
C	62500188610
D	62499613666
E	62499875079
F	62499937801
Total	1000000000000

Table 4.4. Statistics for the first trillion hexadecimal digits of π.
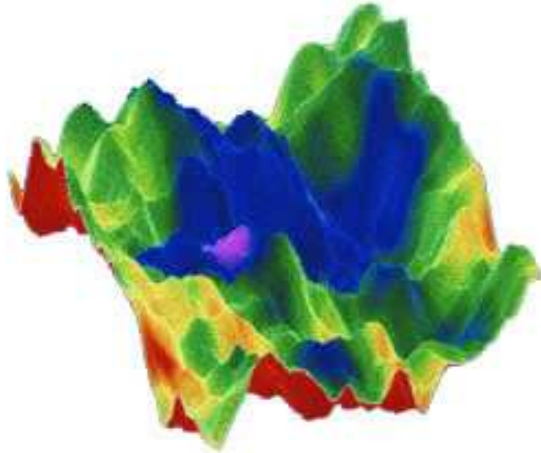
Figure 4.1. A random walk based on one million digits of π (see Color Plate VIII). Courtesy of David and Gregory Chudnovsky.

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 π, 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,

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

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 π, 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 π, 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 π.

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 [171].

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 π (which, of course, is equivalent to the 2-normality of π), 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 [36]. 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 α and β on the unit circumference circle in the natural way. Suppose α is given by a BBP-type formula, namely

$$\alpha = \sum_{k=0}^{\infty} \frac{p(k)}{b^k q(k)}, \tag{4.1}$$

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

$$x_n = \left\{ bx_{n-1} + \frac{p(n)}{q(n)} \right\}, \tag{4.2}$$

where the notation $\{\cdot\}$ denotes the fractional part as before. Recall from Section 3.4 that we can write the base-b expansion of α beginning at position $n + 1$, which we denote α_n, as

$$\alpha_n = \{b^n \alpha\} = \left\{ \sum_{k=0}^{\infty} \frac{b^{n-k} p(k)}{q(k)} \right\}$$

$$= \left\{ \left\{ \sum_{k=0}^{n} \frac{b^{n-k} p(k)}{q(k)} \right\} + \sum_{k=n+1}^{\infty} \frac{b^{n-k} p(k)}{q(k)} \right\}. \tag{4.3}$$

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,

$$||x_n - \alpha_n|| \leq \left| \sum_{k=n+1}^{\infty} \frac{b^{n-k} p(k)}{q(k)} \right|$$

$$\leq \epsilon \sum_{k=n+1}^{\infty} b^{n-k} = \frac{\epsilon}{b - 1} \leq \epsilon. \tag{4.4}$$

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 α be a BBP-type constant as defined above, with α_n the base-b expansion of α beginning at position $n + 1$, and (x_n) the BBP sequence associated with α, 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 α, as given in Formula (4.2), is a close approximation to the sequence (α_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 $0 \le \deg p < \deg q$, and with q having no zeroes for nonnegative integer arguments. Let $b \ge 2$ be an integer, and let $r_n = p(n)/q(n)$. Then the sequence $x = (x_0, x_1, x_2, \cdots)$ determined by the iteration $x_0 = 0$, and*

$$x_n \quad = \quad \{bx_{n-1} + r_n\} \tag{4.5}$$

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 α given by a formula of the type $\alpha = \sum_{k \ge 0} p(k)/(b^k q(k))$, 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

$$x_n \quad = \quad \left\{2x_{n-1} + \frac{1}{n}\right\} \tag{4.6}$$

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

$$x_n = \left\{ 16x_{n-1} + \frac{120n^2 - 89n + 16}{512n^4 - 1024n^3 + 712n^2 - 206n + 21} \right\} \quad (4.7)$$

is equidistributed in $[0, 1)$, then it would follow that π is 16-normal (and so is 2-normal also). This is the BBP sequence for π. The fractional term here is obtained by combining the four fractions in the BBP formula for π, 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 π 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 π. 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 π, 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

$$||\alpha_n - x_n|| \le \sum_{k=n+1}^{\infty} \frac{120k^2 - 89k + 16}{16^{j-n}(512k^4 - 1024k^3 + 712k^2 - 206k + 21)}$$

$$\approx \frac{120(n+1)^2 - 89(n+1) + 16}{16(512(n+1)^4 - 1024(n+1)^3 + 712(n+1)^2 - 206(n+1) + 21)}$$

$$(4.8)$$

so that

$$\sum_{n=1}^{\infty} ||\alpha_n - x_n|| \quad \le \quad 0.01579\ldots. \tag{4.9}$$

For the sake of heuristic argument, let us assume for the moment that the α_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 α_n) can only occur when α_n is within δ_n of one of the points $(0, 1/16, 2/16, \cdots, 15/16)$. 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 [53, 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 1.465×10^{-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 π, $\log 2$, and other BBP-type constants [37]. In the previous section, we noted that the 2-normality of

$$\log 2 \quad = \quad \sum_{n=1}^{\infty} \frac{1}{n2^n} \tag{4.10}$$

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:

$$\alpha_{b,c} \quad = \quad \sum_{n=c^k>1} \frac{1}{nb^n} = \sum_{k=1}^{\infty} \frac{1}{c^k b^{c^k}}, \tag{4.11}$$

where $b > 1$ and $c > 2$ are integers. The simplest instance of this class is

$$\alpha_{2,3} = \sum_{n=3^k>1} \frac{1}{n2^n} = \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k}} \tag{4.12}$$

$$= 0.04188368083150298507125289862457168242609675846654857\ldots_{10}$$

$$= 0.0AB8E38F684BDA12F684BF35BA781948B0FCD6E9E06522C3F35B\ldots_{16}.$$

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 [247] that if $|P/Q - \alpha| < 1/Q^{2+\epsilon}$ admits infinitely many rational solutions P/Q (i.e., if α is approximable to degree $2 + \epsilon$ for some $\epsilon > 0$), then α is transcendental. We show here that $\alpha_{b,c}$ is approximable to degree $c - \delta$. Fix a k and write

$$\alpha_{b,c} \quad = \quad P/Q + \sum_{n>k} \frac{1}{c^n b^{c^n}}, \tag{4.13}$$

where $\gcd(P, Q) = 1$ and $Q = c^k b^{c^k}$. The sum over n gives

$$|\alpha_{b,c} - P/Q| \quad < \quad \frac{2}{c^{k+1}(Q/c^k)^c} \quad < \quad \frac{c^{kc}}{Q^c}. \tag{4.14}$$

Now $c^k \log b + k \log c = \log Q$, so that $c^k < \log Q/\log b$, and we can write

$$c^{kc} \quad < \quad (\log Q/\log b)^c \quad = \quad Q^{c(\log\log Q - \log\log b)/\log Q}. \tag{4.15}$$

Thus for any fixed $\delta > 0$,

$$|\alpha_{b,c} - P/Q| \quad < \quad \frac{1}{Q^{c(1+\log\log b/\log Q - \log\log Q/\log Q)}} \quad < \quad \frac{1}{Q^{c-\delta}}, \tag{4.16}$$

for all sufficiently large k. $\qquad\qquad\square$

Consider now the BBP sequence associated with $\alpha_{2,3}$, namely the sequence defined by $x_0 = 0$, and

$$x_n \quad = \quad \{2x_{n-1} + r_n\}, \tag{4.17}$$

where $r_n = 1/n$ if $n = 3^k$, and $r_n = 0$ otherwise. Successive iterates of this sequence are:

$$0,\ 0,\ 0, \frac{1}{3},\ \frac{2}{3},\ \frac{1}{3},\ \frac{2}{3},\ \frac{1}{3},\ \frac{2}{3},$$

$$\frac{4}{9},\ \frac{8}{9},\ \frac{7}{9},\ \frac{5}{9},\ \frac{1}{9},\ \frac{2}{9},\ \frac{4}{9},\ \frac{8}{9},\ \frac{7}{9},\ \frac{5}{9},\ \frac{1}{9},\ \frac{2}{9},\ \frac{4}{9},\ \frac{8}{9},\ \frac{7}{9},\ \frac{5}{9},\ \frac{1}{9},\ \frac{2}{9},$$

$$\frac{13}{27},\ \frac{26}{27},\ \frac{25}{27},\ \frac{23}{27},\ \frac{19}{27},\ \frac{11}{27},\ \frac{22}{27},\ \frac{17}{27},\ \frac{7}{27},\ \frac{14}{27},\ \frac{1}{27},\ \frac{2}{27},\ \frac{4}{27},\ \frac{8}{27},\ \frac{16}{27},\ \frac{5}{27},\ \frac{10}{27},\ \frac{20}{27},$$

$$\frac{13}{27},\ \frac{26}{27},\ \frac{25}{27},\ \frac{23}{27},\ \frac{19}{27},\ \frac{11}{27},\ \frac{22}{27},\ \frac{17}{27},\ \frac{7}{27},\ \frac{14}{27},\ \frac{1}{27},\ \frac{2}{27},\ \frac{4}{27},\ \frac{8}{27},\ \frac{16}{27},\ \frac{5}{27},\ \frac{10}{27},\ \frac{20}{27},$$

$$\frac{13}{27},\ \frac{26}{27},\ \frac{25}{27},\ \frac{23}{27},\ \frac{19}{27},\ \frac{11}{27},\ \frac{22}{27},\ \frac{17}{27},\ \frac{7}{27},\ \frac{14}{27},\ \frac{1}{27},\ \frac{2}{27},\ \frac{4}{27},\ \frac{8}{27},\ \frac{16}{27},\ \frac{5}{27},\ \frac{10}{27},\ \frac{20}{27}.$$

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 $z_n = 2z_{n-1} \bmod 3^j$ 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

$$\alpha_{b,c} \quad = \quad \sum_{n=c^k>1} \frac{1}{nb^n} \quad = \quad \sum_{k=1}^{\infty} \frac{1}{c^k b^{c^k}}, \tag{4.18}$$

where $b > 1$, and c is co-prime to b, is b-normal. This result was first given in [37]. We present here a significantly simpler proof, based on the following lemma:

Lemma 4.16. (Hot spot lemma). *The constant α is b-normal if and only if there exists a constant M such that for every interval (c, d),*

$$\limsup_{n \to \infty} \frac{\#_{0 \le j < n}[\{b^j \alpha\} \in (c, d)]}{n(d - c)} \quad \le \quad M. \tag{4.19}$$

This result is proved in [195, pg. 77]. A stronger result is given in [39].

Theorem 4.17. *Each of the constants*

$$\alpha_{b,c} \quad = \quad \sum_{k=1}^{\infty} \frac{1}{c^k b^{c^k}}, \tag{4.20}$$

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 α, 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, if $r_k = 1/k$ if $k = 3^r$, and zero otherwise (as above), then

$$|x_n - \{2^n \alpha_n\}| \quad = \quad \left| \sum_{k=n+1}^{\infty} 2^{n-k} r_k \right| \quad < \quad \frac{1}{2n}. \tag{4.21}$$

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 $3^p \le n < 3^{p+1}$. Let $m = \lfloor 1/(d-c) \rfloor + 1$. Now note that for $j \ge m$, 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 $x_j \in D = [c - (d-c)/2, d + (d-c)/2)$. Therefore we can write

$$\frac{\#_{0 \le j < n}(\{2^j \alpha\} \in [c, d))}{n(d-c)} \quad \le \quad \frac{m + \#_{m \le j < n}(x_j \in D)}{n(d-c)}$$

$$\le \quad \frac{m + 3(2 \cdot 3^p (d-c) + 1)}{n(d-c)} \quad < \quad 8.$$

We have shown that for all $[d - c]$,

$$\limsup_{n \ge 1} \frac{\#_{0 \le j < n}(\{2^j \alpha\} \in [c, d))}{n} \quad \le \quad 8(d - c),$$

so by the hot spot lemma, α is 2-normal.   □

We should add that $\alpha_{2,3}$ was actually proven 2-normal by Stoneham in 1970 [266]. 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 [37] that all constants of the form

$$\alpha_{2,3}(r) \quad = \quad \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k + r_k}}, \qquad\qquad (4.22)$$

where r_k is the k-th bit in the binary expansion of $r \in (0, 1)$, are 2-normal and transcendental. It is fairly easy 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 sidelight, these α 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. This 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 $\sqrt{2}$, $\sqrt[3]{10}$ 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 [30]. 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 $(A_k(x, y, n),\ 0 \le k < 2n)$ 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

$$A_k(x, y, n) \quad = \quad \sum_{j=0}^{n-1} x_j y_{k-j}, \qquad\qquad 0 \le k < 2n,$$

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*

$$\liminf_{n\to\infty} \frac{B_n(s)}{\sqrt{C(r)n}} \quad \ge \quad 1,$$

We first prove two lemmas.

Lemma 4.19. *For any two positive integers a and b, $B(a + b) \le B(a) + B(b)$, and $B(ab) \le B(a)B(b)$. The same is true for reals, namely $B_n(x + y) \le B_n(x) + B_n(y)$ and $B_n(xy) \le B_n(x)B_n(y)$, 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. $\square$

Lemma 4.20. *For x and y with $0 < x, y < 1$, define*

$$z_n(x, y) \quad = \quad \sum_{k=0}^{2n-1} A_k(x, y, n) 2^{-k-1}. \tag{4.23}$$

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 α_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

$$|z_n(x, y) - xy| \quad < \quad \alpha_n \delta_n + \gamma_n \beta_n + \beta_n \delta_n \quad < \quad 2 \cdot 2^{-n} \quad = \quad 2^{1-n}. \tag{4.24}$$

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 $B_n(z_n(s, s)) \leq B_n^2(s)$. Now since $z_n(s, s)$ replicates with increasing fidelity the expansion of r, we must have, at the least,

$$\liminf_{n \to \infty} \frac{B_n(z_n(s, s))}{n} \quad = \quad \liminf_{n \to \infty} \frac{B_n(r)}{n}. \tag{4.25}$$

But since $B_n(r)/n$ converges to $C(r)$, this means that given $\epsilon > 0$,

$$n(B_n(s)/n)^2 \geq B_n(z_n(s,s))/n \;\geq\; B_n(r)/n - \epsilon \;\geq C(r) - 2\epsilon \quad (4.26)$$

for all sufficiently large n, which establishes our result. $\square$

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 ϵ) 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 [30]. 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 [36], 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 α and

β on the unit circumference circle in the natural way. A simple result, which we will term the "dilated-norm rule," is the following: If $0 \le \delta \le 1/(2||z||)$, 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 α_j is an integer in $[0, b-1]$, is taken to be unique for α. 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 α to be the limit as $N \to \infty$ of the number of instances where $\alpha_j = d_1$, $\alpha_{j+1} = d_2$, $\cdots$, $\alpha_{j+k-1} = d_k$, $j \le N + 1 - k$, divided by N.

For a sequence $x = (x_0, x_1, \cdots)$ of real numbers in $[0, 1)$, we define the counting function

$$C(x, c, d, N) \quad = \quad \#(x_j \in [c, d) \ : \ j < N).$$

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 $0 \le c < d < 1$ we have*

$$\lim_{N \to \infty} \frac{C(x, c, d, N)}{N} \quad = \quad d - c.$$

This definition is identical to that of "uniform distribution modulo 1," as given in [195, 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 β) 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 α 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 $k \ge 0$, we have $||x_{K+k} - w_{t(k)}|| < \epsilon$, for some function $t(k)$, with $0 \le t(k) < P$.*

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 β 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 ϵ-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 α be real and assume an integer base $b \geq 2$. If the sequence $x = (\{b^n \alpha\})$ has a finite attractor W, then W is a periodic attractor, and the structure of the attractor W is necessarily*

$$W \quad = \quad (w_0, \{bw_0\}, \{b^2 w_0\}, \cdots, \{b^{P-1} w_0\}).$$

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 $d = \min_{0 \leq i, j < P}(\|w_i - w_j\|)$, and choose $\epsilon < d/(4b)$. Let W_ϵ 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 $x_k \in W_\epsilon$. Let K be the first $k > K'$, such that $\|x_k - w_0\| < \epsilon$. We then have:

$$\|x_{K+1} - bw_0\| \quad = \quad \|bx_K - bw_0\| = b\|x_K - w_0\| < b\epsilon < d/4, \quad (4.27)$$

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 $b\epsilon$ of $\{bw_0\}$, and similarly x_{K+k+1} is within $b\epsilon$ of $\{bw_0\}$ whenever x_{K+k} is within ϵ 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 ϵ 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 $w_2 = \{b^2 w_0\}$, 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 ϵ region around w_0 would never be visited again by the x sequence and thus w_0 could not be a member of

the attractor set. Therefore, $W = (w_0, \{bw_0\}, \cdots, \{b^{P-1}w_0\})$, 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 $W = \{w_0, w_1, \cdots, w_{P-1}\}$ be the finite attractor for x. Let $d = \min_{0 \le i,j < P}(||w_i - w_j||)$, and choose $\epsilon < d/(4b+4)$. Let W_ϵ be the set of all z in $[0,1)$ such that $||z - w_i|| < \epsilon$ for some $0 \le i < P$. 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):

$$\begin{aligned} ||x_{K+1} - bw_0|| &= ||bx_K + r_{K+1} - bw_0|| \le b||x_K - w_0|| + \epsilon \\ &< (b+1)\epsilon < d/4. \end{aligned} \tag{4.28}$$

The remainder of the proof of this result follows the second paragraph of the proof of Theorem 4.0.   □

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 α 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 $m = \lfloor \log_b(\epsilon/h) \rfloor$, and note that $b^m h \le \epsilon < b^{m+1}h < b\epsilon < 1/4$. Thus we can write (once again using the dilated-norm rule):

$$\begin{aligned} ||x_{K+m+1} - w_{m+1 \mod P}|| &= ||b^{m+1}x_K - b^{m+1}w_0|| = b^{m+1}||x_K - w_0|| \\ &= b^{m+1}h > \epsilon. \end{aligned} \tag{4.29}$$

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 $k \ge 0$. In other words, after at most K initial digits, the base-b expansion of α repeats with period P, so that α is rational. As for the converse, $\alpha = p/q$ rational implies

the sequence $(b^n p/q) = (((pb^n) \mod q)/q)$ 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. $\square$

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 α possesses a formula of the form

$$\alpha = \sum_{k=1}^{\infty} \frac{1}{b^k} \frac{p(k)}{q(k)}, \tag{4.30}$$

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 α is rational if and only if the sequence (x_n), where

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

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 α is rational. Following the BBP strategy, we can write

$$\{b^n \alpha\} = \left\{ \sum_{k=1}^{n} \frac{b^{n-k} p(k)}{q(k)} + \sum_{k=n+1}^{\infty} \frac{b^{n-k} p(k)}{q(k)} \right\} \tag{4.31}$$

$$= \{x_n + t_n\}, \tag{4.32}$$

where x is defined by $x_0 = 0$ and the recursion

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

with the sequence t given by

$$t_n = \sum_{k=1}^{\infty} \frac{1}{b^k} \frac{p(k+n)}{q(k+n)}.$$

Provided that $\deg p < \deg q$ as in Hypothesis 4.0, given any ϵ there is some n such that $|p(k+n)/q(k+n)| < \epsilon$ for all $k \geq 1$. For such n, we have $|t_n| < \epsilon \sum_{k \geq 1} b^{-k} = \epsilon/(b-1) \leq \epsilon$. 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 α is rational. $\square$

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 $\limsup_n A_n(= \cup_n \cap_{m>n} A_m) = 0$.

   (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 ω. Note that $s_n(\omega)/n \to 0$ if and only if $\sum_{k \le n} d_k(\omega)/n \to 1/2$. Show for $\varepsilon > 0$ that

   $$P[\omega : |s_n(\omega)| \ge n\varepsilon] \le \frac{1}{n^4 \varepsilon^4} \int_0^1 s_n^4 \, d\omega.$$

   Then show that

   $$\int_0^1 s_n^4 \, d\omega = n + 3n(n-1)$$

   and deduce the $P[\omega : |s_n(\omega)| \ge n\varepsilon] \le 3/(n^2 \varepsilon^4)$. If we choose ε_n appropriately $\sum_n P[\omega : |s_n(\omega)| \ge n\varepsilon_n]$ is finite. Conclude that $s_n(\omega)/n \to 0$ for almost all ω 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 [47]. 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 $\limsup_n A_n = 1$. Together they provide a "zero-one" law. Full details are in [53].

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 nth 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 [74, pg. 352].

3. **Rational times normal is normal.**

   Theorem 4.31. *Whenever α 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 α is normal, and consider $p\alpha$ for a positive integer p. Let $\{\cdot\}$ denote fractional part. Then $\{b^j p\alpha\} \in [x, y)$ implies that one of the following p mutually exclusive conditions must hold:

   $$\begin{aligned}
   \{b^j \alpha\} &\in [x/p, \ y/p) \\
   \{b^j \alpha\} &\in [x/p + 1/p, \ y/p + 1/p) \\
   \{b^j \alpha\} &\in [x/p + 2/p, \ y/p + 2/p) \\
   &\cdots \qquad \cdots \\
   \{b^j \alpha\} &\in [x/p + (p-1)/p, \ y/p + (p-1)/p).
   \end{aligned}$$

   Since α is normal, the limiting frequency of each of the above is $(y - x)/p$. Thus the limiting frequency of $\{b^j p\alpha\} \in [x, y)$ is p times this value, or $y - x$. This establishes that $p\alpha$ is normal.

   Now suppose that α is normal, and consider α/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

$$\limsup_{n\to\infty} \frac{\#_{0\leq j\leq n-1}(\{b^j\alpha/p\}\in[x,\gamma))}{n} \quad \leq \quad p(\gamma-x),$$

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 α/p is normal. This proof is taken from [41]. See also exercise 8.9 in [195, pg. 77].   □

4. **Rational plus normal is normal.**

Theorem 4.32. *Whenever α 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:

$$U_d(R) = \sum_{m=1}^{\infty} \frac{\binom{R+m+d-1}{d-1}}{2^m} \qquad (r, D \in \mathrm{N}).$$

(a) It is easy to discover that $U_d(R)$ satisfies the recursion

$$f(R, d) - 2f(R, d-1) = \binom{R+d-1}{d-1}. \qquad (4.33)$$

Now *Maple* can "tell" one that

$$U_d(R) = \frac{1}{2} \binom{R+d}{d-1} \mathrm{F}\left(1, d+R+1, R+2; \frac{1}{2}\right), \qquad (4.34)$$

and a computer-algebra-assisted use of Euler's integral for the hypergeometric function simplifies to

$$\sum_{m=1}^{\infty} \frac{\binom{R+m+d-1}{d-1}}{2^m} = \frac{\int_0^1 (2-x)^{d-1} x^R \, dx}{\beta(R+1, d)} \qquad (4.35)$$

(the β 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

$$\mathcal{K}(R,d) \;=\; \int_0^1 (2-x)^{d-1}\, x^R\, dx, \qquad (4.36)$$

so that

$$V_d(R) \;=\; \frac{\mathcal{K}(R,d)}{\beta\,(R+1,d)}. \qquad (4.37)$$

Observe with a change of variables

$$\frac{1}{R+1} \;<\; \mathcal{K}(R,d) = \int_0^1 (1+t)^{d-1}\,(1-t)^R\, dt$$

$$= \int_0^1 \left(1-t^2\right)^{d-1}\,(1-t)^{R+1-d}\, dt$$

$$< \int_0^1 (1-t)^{R+1-d}\, dt = \frac{1}{R+2-d},$$

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

$$\frac{R}{R+2} \le \gamma_d(R) < \left(1+\frac{1}{m}\right) e^{\frac{1}{m+1}}$$

for $R > m\,d, m \ge 1$. 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

$$\limsup_{R\to\infty} \frac{U_d(R)}{\left(R^{(d-1)}/(d-1)!\right)} \le 1.$$

We leave it to the reader to show, using Stirling's formula, that indeed

$$\lim_{R \to \infty} \frac{U_d(R)}{\left(R^{(d-1)}/(d-1)!\right)} = 1.$$

(c) Show that

$$U_d(R) = \sum_{j=0}^{d-1} \binom{R+d}{j}.$$

See [30] for further details.

7. **Sierpinski's number.** As noted in this chapter, in 1916 Sierpinski gave an "effective" construction of an absolutely normal number, σ, recently expressed recursively in [47]. That said, the present algorithm does not allow computation of any digits of σ. 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

$$x_n = \frac{2^{n-m} \lfloor m/2 \rfloor \bmod m}{m}.$$

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 $x_{53(n+1)} = qx_{53n} \bmod m$, 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 $a \le j < a + n$ 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. *Hint*: See [187, 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 pseudo-random 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. *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

0000001000000100000110001000011010001111110010111011101000010000,

as has been recently established in [99].

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

$$\left| \frac{p}{q} - \sum_{n=0}^{q} \frac{1}{n!} \right| < \frac{1}{q \cdot q!}.$$

   (c) More generally, prove that $\sum_{n \geq 0} (\pm 1)_n / n!$ is irrational for all choices of $(\pm 1)_n$, thus explicitly constructing continuum-many irrational numbers.

   (d) Establish *Liouville's theorem* that if α is algebraic of degree n, then for all $\varepsilon > 0$ and all $c > 0$

$$0 < \left| \alpha - \frac{p}{q} \right| < \frac{c}{q^{n+\varepsilon}}$$

   has only finitely many solutions with p and q integer.

   (e) Deduce that $\sum_{n \geq 0} (\pm 1)_n / 10^{n!}$ 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 $0.23571113171923\ldots$, 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* [192]:

> 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 few 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 astonishing legacy in a field where a lifetime product of 50 papers is considered extraordinary.

Mathematicians tend to bloom early and die early. The great Indian 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 literally 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.
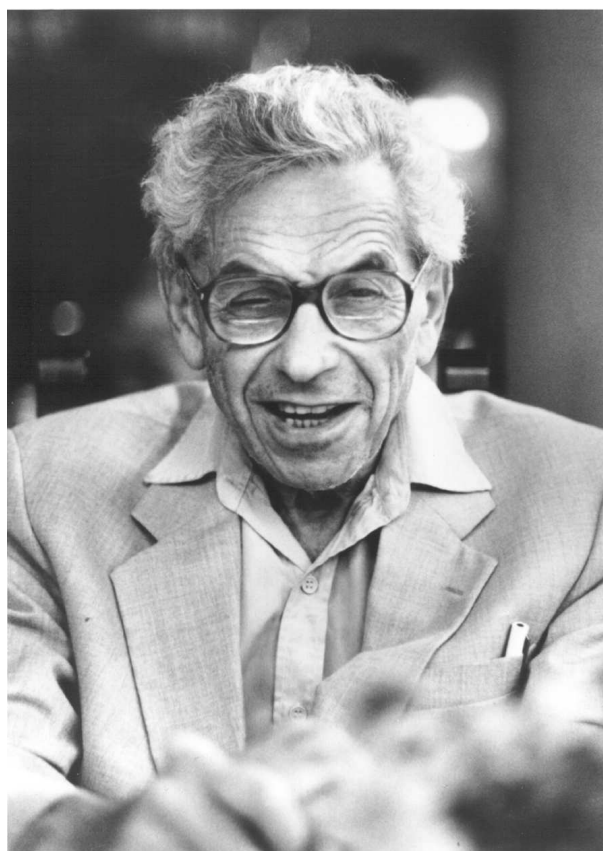
Figure 4.2. A 1993 photo of Paul Erdős. Photograph of Paul Erdos by George Csicsery from his documentary film "N is a Number: A Portrait of Paul Erdos" (1993).

5 | The Power of Constructive Proofs I

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 C:

$$p(x) \quad = \quad a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n. \tag{5.1}$$

Suppose that $p(x)$ has no roots in 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

$$q(z) \quad = \quad p(z - t) \; = \; q_0 + q_1 z + \cdots + q_n z^n. \tag{5.2}$$

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

$$x_{k+1} \quad = \quad x_k - \frac{f(x_k)}{f'(x_k)} \tag{5.3}$$

(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

$$x_{k+1} \quad = \quad x_k + \left(\frac{-m! f(x_k)}{f^{(m)}(x_k)} \right)^{1/m}, \tag{5.4}$$

where the m-th root of a complex number $z = ae^{ib}$ is calculated using the well-known formula

$$z^{1/m} \quad = \quad a^{1/m} \left(\cos(b/m) + i \sin(b/m) \right). \tag{5.5}$$

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):

$$q(x) \quad = \quad q_0 + q_m x^m + q_{m+1} x^{m+1} + \cdots + q_n x^n. \tag{5.6}$$

Note that $q^{(m)}(x) = m! q_m$. Thus, in accordance with (5.4), we will choose x to be the complex number

$$x \quad = \quad r \left(\frac{-q_0}{q_m} \right)^{1/m} \tag{5.7}$$

for some small positive real r that we will specify below. Now we can write

$$
\begin{aligned}
q(x) &= q_0 - q_0 r^m + q_{m+1} r^{m+1} \left(\frac{-q_0}{q_m}\right)^{1+1/m} + \cdots + q_n r^n \left(\frac{-q_0}{q_m}\right)^{n/m} \\
&= q_0(1 - r^m) + \mathcal{E},
\end{aligned}
\tag{5.8}
$$

where the error term $\mathcal{E}$ satisfies

$$
|\mathcal{E}| \leq \frac{r^{m+1} \max |q_i|}{1-s} \left|\frac{q_0}{q_m}\right|^{1+1/m}
\tag{5.9}
$$

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 σ 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

$$|q(z)| \;\leq\; a\,|z| + b, \text{ when } -1/2 \leq \operatorname{Re}(z) \leq 1/2 \tag{5.14}$$

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

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

$$\inf_{|x|,|y| \leq 1/2} \left| \frac{\sin z}{z} \right| > 0 \qquad (5.15)$$

as sin has zeroes only at the integers, while for $|x| \leq 1/2$ and $|y| \geq 1/2$ we have

$$|\sin(\pi z)| \geq |\sinh(\pi|y|)| \geq c \exp(\pi|z|) - d, \qquad (5.16)$$

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

$$\sqrt{-x} \to i\sqrt{x}\,,$$

and therefore when it tried substituting, say, $x = -4$ it computed as follows.

$$\sqrt{-x} \quad \to i\sqrt{x}; \qquad i\sqrt{x} \quad \to i\sqrt{-4}; \qquad i\sqrt{-4} \quad \to i^2\sqrt{4} \to -2\,.$$

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(ASIN(5/4))` $\rightarrow -5/4$ using the "standard" formulae:

$$\arcsin z \quad = \quad \arctan\left(\frac{z}{\sqrt{1-z^2}}\right) \qquad (5.17)$$

$$\sin\left(\arctan z\right) \quad = \quad \frac{z}{\sqrt{z^2+1}}, \qquad (5.18)$$

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

$$\arcsin z \quad = \quad \arctan\left(\frac{z}{\sqrt{1-z^2}}\right)$$

$$\sin\left(\arctan z\right) \quad = \quad \frac{z}{\sqrt{z^2+1}} = z\frac{1}{\sqrt{z^2+1}}$$

to

$$\arcsin z \quad = \quad \arctan\left(\frac{z}{\sqrt{1-z^2}}\right) \qquad (5.19)$$

$$\sin\left(\arctan z\right) \quad = \quad z\sqrt{\frac{1}{z^2+1}}, \qquad (5.20)$$

and to ensure that

$$\sqrt{\frac{1}{z}} \text{ was } not \text{ automatically simplified to } \frac{1}{\sqrt{z}}.$$

□

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

$$\sqrt{xy} \;\; \to \;\; \sqrt{x}\sqrt{y}, \qquad \sqrt{x^2} \to x,$$

$$\sqrt{\frac{1}{z}} \;\; \to \;\; \frac{1}{\sqrt{z}}, \qquad\qquad \log(e^z) \to z,$$

$$\log(1/z) \;\; \to \;\; -\log z, \qquad \arctan z = \arcsin\left(\frac{z}{\sqrt{z^2+1}}\right),$$

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 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

$$\mathrm{Log}(AB) = \mathrm{Log}A + \mathrm{Log}B;$$

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 *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 *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 *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 $\{i\pi + 2i\pi k \mid k \in \mathbb{Z}\}$? Some object in between these two, perhaps a single number $i\pi + 2i\pi k$ 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

$$z = \left(r + \left(r^2 + q^3\right)^{1/2}\right)^{1/3} + \left(r - \left(r^2 + q^3\right)^{1/2}\right)^{1/3} \ .$$

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 symmetry, z is elected from a set of *more than three* possible z.

Jeffrey writes:

> Traditionally, this inefficiency has not bothered human mathematicians, 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*, [175, 113], to keep transformations correct. In conclusion he appropriately notes that there is reluctance to give up the old formulae

$$\left(\left(\left(\left(\left(z^2\right)^{1/2}\right)^3\right)^{1/3}\right)^4\right)^{1/4} = z \ ??$$

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 [112] 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 quantum mechanics, which is often expressed as the fact that the position and momentum of a subatomic-scale particle cannot simultaneously be prescribed 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 Δt is short enough, the perceived pitch would be ambiguous, so that the "uncertainty" in the frequency Δf 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 Δf 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):

$$
\begin{aligned}
E(f) &= \int_{-\infty}^{\infty} f^2(t)\, dt \\
V(f) &= \int_{-\infty}^{\infty} t^2 f^2(t)\, dt \\
\hat{f}(x) &= \int_{-\infty}^{\infty} f(t) e^{-itx}\, dt \\
Q(f) &= \frac{V(f)}{E(f)} \cdot \frac{V(\hat{f})}{E(\hat{f})}.
\end{aligned}
\tag{5.22}
$$

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 [5, pg. 256] (see also formula (5.32)), to the functions $tf(t)$ and $f'(t)$, we can write

$$
\left| \int_{-\infty}^{\infty} t f(t) f'(t)\, dt \right|^2 \leq \left[\int_{-\infty}^{\infty} t^2 f^2(t)\, dt \right] \left[\int_{-\infty}^{\infty} (f'(t))^2 dt \right]. \tag{5.23}
$$

Furthermore,

$$\int_{-\infty}^{\infty} tf(t)f'(t)\,dt \;\;=\;\; \frac{1}{2}\int_{-\infty}^{\infty} t\frac{df^2(t)}{dt}\,dt \;\;=\;\; -\frac{1}{2}E(f) \qquad (5.24)$$

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 [228, pg. 65] to $f(t)$ and $g(t)$, we obtain, respectively,

$$\int_{-\infty}^{\infty} |f(t)|^2\,dt \;\;=\;\; \frac{1}{2\pi}\int_{-\infty}^{\infty} |\hat{f}(x)|^2\,dx$$

$$\int_{-\infty}^{\infty} |f'(t)|^2\,dt \;\;=\;\; \frac{1}{2\pi}\int_{-\infty}^{\infty} x^2|\hat{f}(x)|^2\,dx. \qquad (5.25)$$

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 $f(t)$. $\qquad\square$

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

$$Q(f) \;\;=\;\; \frac{V(f)}{E(f)} \cdot \frac{V(\hat{f})}{E(\hat{f})}. \qquad (5.26)$$

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

$f(t)$	Interval	$\hat{f}(x)$	$E(f)$	$V(f)$	$V(\hat{f})$	$Q(f)$
$1 - t\,\mathrm{sgn}t$	$[-1,1]$	$2(1-\cos x)/x^2$	$2/3$	$1/15$	4π	$3/10$
$1-t^2$	$[-1,1]$	$4(\sin x - x\cos x)/x^3$	$16/15$	$16/105$	$16\pi/3$	$5/14$
$1/(1+t^2)$	$[-\infty,\infty]$	$\pi\exp(-x\,\mathrm{sgn}x)$	$\pi/2$	$\pi/2$	$\pi^2/2$	$1/2$
$e^{-|t|}$	$[-\infty,\infty]$	$2/(1+x^2)$	1	$1/2$	2π	$1/2$
$1+\cos t$	$[-\pi,\pi]$	$2\sin(\pi x)/(x-x^3)$	3π	$\pi^3-15\pi/2$	$2\pi^2$	$(\pi^2-15/2)/9$

Table 5.1. Q values for various functions.

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

$$\hat{f}\left(\frac{bk}{n}\right) = \int_{-\infty}^{\infty} f(t)e^{-itbk/n}\,dt$$

$$\approx \frac{a}{n}\sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} f\left(\frac{aj}{n}\right)e^{-i(aj/n)(bk/n)} \tag{5.27}$$

$$= \frac{a}{n}\sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} f\left(\frac{aj}{n}\right)e^{-2\pi ijk/n} \tag{5.28}$$

for $-n/2 + 1 \le k \le n/2$. 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

$$\hat{f}\left(\frac{bk}{n}\right) = \frac{a}{n}\sum_{j=0}^{n-1} f\left(\frac{aj}{n}\right)e^{-2\pi ijk/n}, \tag{5.29}$$

for $0 \le k \le n - 1$, 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:

$$
E(f) = \int_{-\infty}^{\infty} f^2(t)\, dt \approx \frac{a}{n} \sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} f^2\left(\frac{aj}{n}\right)
$$

$$
V(f) = \int_{-\infty}^{\infty} t^2 f^2(t)\, dt \approx \frac{a}{n} \sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} \left(\frac{aj}{n}\right)^2 f^2\left(\frac{aj}{n}\right)
$$

$$
E(\hat{f}) = \int_{-\infty}^{\infty} \hat{f}^2(x)\, dx \approx \frac{b}{n} \sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} \hat{f}^2\left(\frac{bj}{n}\right)
$$

$$
V(\hat{f}) = \int_{-\infty}^{\infty} x^2 \hat{f}^2(x)\, dx \approx \frac{b}{n} \sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} \left(\frac{bj}{n}\right)^2 \hat{f}^2\left(\frac{bj}{n}\right), \quad (5.30)
$$

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 δ to be some small value, and calculate $Q_{min} = Q(f)$, 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 δ (leaving other y_j unchanged) and calculate $Q(f)$ for $f(t)$ associated with this altered y array. If $Q(f) < Q_{min}$, then replace Q_{min} by $Q(f)$, and replace the y array with the altered y array; if not, then decrease y_k by δ, and replace as before if $Q(f) < Q_{min}$. Either way, increment k and perform similar tests until the case $k = m$ is complete. If for some k the test $Q(f) < Q_{min}$ was true, then repeat beginning with $k = 1$. If not, then reduce δ by a factor of two and start again. Terminate when δ is sufficiently small. $\qquad\square$

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 $e^{-(bt)^2/2}$, 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 $ae^{-(bt)^2/2}$), 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 [12, 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
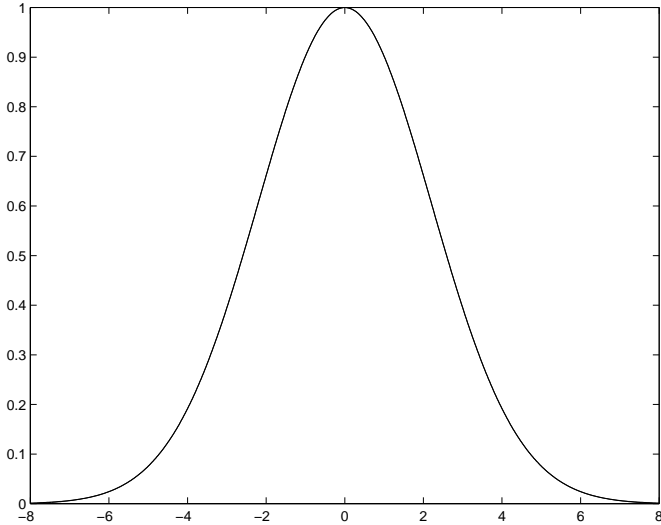
Figure 5.1. Experimental Q-minimizing function and matching Gaussian.
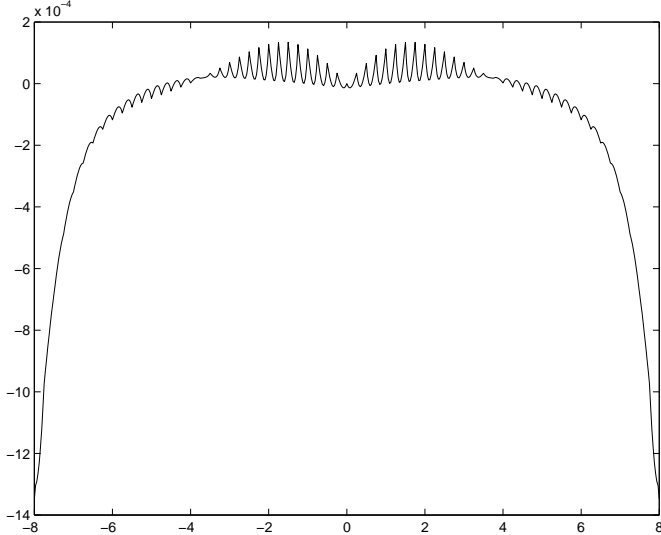
Figure 5.2. Difference between Q-minimizing function and matching Gaussian.

inequality. For $1 \leq p, q \leq \infty$, we define the $p-$norm of a sequence in R^n

$$\|x\|_p \quad = \quad \sqrt[p]{\sum_{k=1}^{n} |x_k|^p}.$$

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*

$$\langle x, y \rangle \quad \leq \quad \|x\|_p \|y\|_q, \tag{5.31}$$

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*

$$\frac{1}{p} |x|^p + \frac{1}{q} |y|^q \quad \geq \quad xy$$

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

$$\sum_k \left(\frac{1}{p} x_k^p + \frac{1}{q} y_k^q \right) \quad \geq \quad \sum_k x_k y_k,$$

which is

$$\frac{1}{p} \|x\|_p^p + \frac{1}{q} \|y\|_q^q \quad \geq \quad \langle x, y \rangle.$$

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

$$\int_R x(t) y(t)\, dt \quad \leq \quad \left[\int_R |x(t)|^p\, dt \right]^{1/p} \left[\int_R |y(t)|^q\, dt \right]^{1/q} \tag{5.32}$$

is proven in the same way.

When $p = q = 2$, we recover the Cauchy-Schwarz inequality. In general for a function $f : \mathrm{R}^n \mapsto \mathrm{R} \cup \infty$, we may define the *(Fenchel-Legendre) conjugate* by

$$f^*(y) \quad = \quad \sup_x \langle x, y \rangle - f(x).$$

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 $f = f^{**}$, [78]. 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

```
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 [78].

(a) Given real $\gamma_1, \gamma_2, \cdots, \gamma_n > 0$, define $h : \mathrm{R}^n \to (-\infty, +\infty]$ by

$$h(x) = \begin{cases} \prod_{i=1}^n x_i^{-\gamma_i} & \text{if } x \in \mathrm{R}_{++}^n \\ +\infty & \text{otherwise.} \end{cases}$$

By writing $g(x) = \exp(\log g(x))$ and using a composition formula, one can prove that

$$h^*(y) = \begin{cases} -(\gamma + 1) \prod_{i=1}^n \left(\dfrac{-y_i}{\gamma_i} \right)^{\gamma_i/(\gamma+1)} & \text{if } -y \in \mathrm{R}_+^n \\ +\infty & \text{otherwise,} \end{cases}$$

where $\gamma = \sum_i \gamma_i$.

(b) Given real $\alpha_1, \alpha_2, \cdots, \alpha_n > 0$, define $\alpha = \sum_i \alpha_i$ and suppose a real μ satisfies $\mu > \alpha + 1$. Now define a function $f : \mathrm{R}^n \times \mathrm{R} \to (-\infty, +\infty]$ by

$$f(x, s) = \begin{cases} \mu^{-1} s^\mu \prod_i x_i^{-\alpha_i} & \text{if } x \in \mathrm{R}_{++}^n, \ s \in \mathrm{R}_+ \\ +\infty & \text{otherwise.} \end{cases}$$

Using part (a) one may then prove that

$$f^*(y,t) = \begin{cases} \rho\nu^{-1}t^\nu \prod_i(-y_i)^{-\beta_i} & \text{if } -y \in \mathrm{R}^n_{++}, \ t \in \mathrm{R}_+ \\ +\infty & \text{otherwise} \end{cases}$$

for constants

$$\nu = \frac{\mu}{\mu - (\alpha + 1)}, \quad \beta_i = \frac{\alpha_i}{\mu - (\alpha + 1)}, \quad \rho = \prod_i \left(\frac{\alpha_i}{\mu}\right)^{\beta_i}.$$

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 Γ-*function* is usually defined as an integral

$$\Gamma(x) \quad = \quad \int_0^\infty \exp(-t)t^{x-1}\,dt \tag{5.33}$$

for $\mathrm{Re}(x) > 0$.

Theorem 5.42. (Bohr-Mollerup). *The $\Gamma-$function is the unique function $f : (0,\infty) \to (0,\infty)$ with the following three properties:*

1. $f(1) = 1$;

2. $f(x + 1) = xf(x)$;

3. *f is log-convex (i.e., $x \to \log(f(x))$ 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

$$\sqrt{\Gamma(x)\,\Gamma(y)} \quad \geq \quad \Gamma\left(\frac{x+y}{2}\right).$$

Conversely, we set $g(x) = \log(f(x))$, we observe that $g(n+1) = \log(n!)$, and use the convexity estimate

$$x \log(n) \quad \leq \quad g(n+1+x) - g(n+1) \quad \leq \quad x \log(n+1) \qquad (5.34)$$

for $0 < x \leq 1$.

Hence, for $0 < x \leq 1$,

$$0 \quad \leq \quad g(x) - \log \frac{n! \, n^x}{x(x+1) \cdots (x+n)} \quad \leq \quad x \log \left(x + \frac{1}{n} \right). \quad (5.35)$$

It follows using $f(x+1) = xf(x)$, that *for all $x > 0$*

$$f(x) \quad = \quad \lim_{n \to \infty} \frac{n! \, n^x}{x(x+1) \cdots (x+n)} \quad = \quad \Gamma(x). \qquad (5.36)$$

$\square$

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*

$$\lim_{n \to \infty} \frac{f(t+n+1)}{n! \, n^t} \quad = \quad 1 \qquad (5.37)$$

for $0 \leq t < 1$, then $f = \Gamma$ on $(a, \infty]$.

Proof. The fact that Γ 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 Γ, on $(a, \infty]$. $\square$

We illustrate the use of the Bohr-Mollerup Theorem as follows:

Example 5.44. The β−function.

The β−function is defined by the integral

$$\beta(x, y) \quad = \quad \int_0^1 t^{x-1} (1-t)^{y-1} \, dt \qquad (5.38)$$

for $\operatorname{Re}(x), \operatorname{Re}(y) > 0$. 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):

$$\beta(x,y) \;=\; \frac{\Gamma(x)\,\Gamma(y)}{\Gamma(x+y)}. \tag{5.39}$$

This we shall now deduce from the Bohr-Mollerup result. We define $f = x \to \beta(x,y)\,\Gamma(x+y)/\Gamma(y)$ 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

$$\Gamma\left(\frac{1}{2}\right) \;=\; \sqrt{\beta\left(\frac{1}{2},\frac{1}{2}\right)} \;=\; \sqrt{\pi}, \tag{5.40}$$

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 R^n. □

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. □

Example 5.46. The sin-product formula.

$$\sin(\pi x) \;=\; \pi x \prod_{n=1}^{\infty} \left(1 - \frac{x^2}{n^2}\right) \tag{5.41}$$

and

$$\frac{\pi}{\sin(\pi x)} \quad = \quad \Gamma(x)\Gamma(1-x). \tag{5.42}$$

Now (5.42) follows directly from (5.41) and (5.36). We outline a proof of (5.41) whose full details are in [268]. We examine the polynomial

$$P_m(x) \quad = \quad \frac{1}{2i}\left[\left(1+\pi i\frac{x}{m}\right)^m - \left(1-\pi i\frac{x}{m}\right)^m\right] \to_m \sin(\pi x),$$

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 π, we may write

$$P_{2m}(x) \quad = \quad x\prod_{j=1}^{k-1}\left(1-\frac{\pi^2 x^2}{4k^2\tan^2(j\pi/(2k))}\right). \tag{5.43}$$

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 $x \to 0$. $\qquad\square$

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

$$\frac{\sin(\pi x)}{x} \quad = \quad c\prod_{n=1}^{\infty}\left(1-\frac{x^2}{n^2}\right), \tag{5.44}$$

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

$$V_n(p) \quad = \quad 2^n\frac{\Gamma(1+\frac{1}{p})^n}{\Gamma(1+\frac{n}{p})}, \tag{5.45}$$

([6], Section 1.8). We note that the Γ-function again proves invaluable, and that even the special case when $p = 2$,

$$V_n \quad = \quad 2^n\frac{\Gamma(\frac{3}{2})^n}{\Gamma(1+\frac{n}{2})} \quad = \quad \frac{\Gamma(\frac{1}{2})^n}{\Gamma(1+\frac{n}{2})},$$

gives a formula more concise than that recorded in most analysis books. One can try graphing this as a function of p for $n = 2, 3, \cdots$, 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.

```
vol := proc(n)
  local f,x,i,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

$$L(z) \quad = \quad L(f)(z) \quad = \quad \int_0^\infty e^{-zt} f(t)\, dt$$

for $\operatorname{Re}(z) > 0$. We finish the section with another, induction-free, Laplace transform-based, proof of (5.45). We shall evaluate

$$v_p(y) \quad = \quad \operatorname{Vol}_n(\{x : \|x\|_p^p \le y\}),$$

for $y > 0$ as follows. First, observe that

$$v_p(y) \quad = \quad v_p(1)\, y^{n/p}.$$

We now compute

$$L(v_p)(1) \quad = \quad v_p(1)\, L(y \mapsto y^{n/p})(1) \quad = \quad v_p(1)\, \Gamma\left(1 + \frac{n}{p}\right). \quad (5.46)$$

To evaluate the left-hand side we write

$$
\begin{aligned}
L(v_p)(1) \;&=\; \int_0^\infty e^{-t}\left(\int_{\|x\|_p^p \le t} dx\right) dt \\
&=\; \int_{\mathrm{R}}\left(\int_{\|x\|_p^p}^\infty e^{-t}\,dt\right) dx \;=\; \int_{\mathrm{R}^{\mathbf{n}}} e^{-\|x\|_p^p}\,dx \\
&=\; \prod_{k=1}^n \int_{\mathrm{R}} e^{-|x_k|^p}\,dx_k \;=\; 2^n\,\Gamma\left(1+\frac{1}{p}\right)^n. \qquad (5.47)
\end{aligned}
$$

Now comparing (5.46) and (5.47) recovers

$$
v_p(1) \;=\; 2^n\,\frac{\Gamma(1+\frac{1}{p})^n}{\Gamma(1+\frac{n}{p})}
$$

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 Γ function.

Theorem 5.47.

$$
\lim_{n\to\infty}\frac{n!}{\sqrt{2\pi n}\,(n/e)^n} = 1 \qquad (5.48)
$$

and moreover, for $n > 1$

$$
1+\frac{1}{12n+12} < \frac{n!}{\sqrt{2\pi n}\,(n/e)^n} < 1+\frac{1}{12n-24}. \qquad (5.49)
$$

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

$$
\begin{aligned}
n \log(n) - n + 1 &= \sum_{k=1}^{n-1} \int_k^{k+1} \log(x)\, dx \\
&= \frac{1}{2} \sum_{k=1}^{n-1} \left[\log(k) + \log(k+1) \right] \\
&\quad + \frac{1}{12} \sum_{k=1}^{n} e_k^{-2},
\end{aligned}
\tag{5.50}
$$

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 $(n + 1/2) \log(n) - n - \log(n!) \to R - 1$, or equivalently that $r_n = n^{-n-1/2} \exp(n)\, n!$ converges to a limit r, and so also

$$
r \;=\; \lim_{n \to \infty} \frac{r_n^2}{r_{2n}} \;=\; \lim_{n \to \infty} \frac{\Gamma(n+1)^2\, 4^n \sqrt{2}}{\Gamma(2n+1)\, \sqrt{n}}.
\tag{5.51}
$$

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 π (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 $\binom{2n}{n} \sim 4^n / \sqrt{\pi n}$, 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

$$f(x) \;=\; \left(\int_0^x e^{-s^2}\, ds \right)^2$$

$$g(x) \;=\; \int_0^1 \frac{\exp(-x^2(1+t^2))}{1+t^2}\, dt.$$

The derivative of $f + g$ is zero: In *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 $0 \le s \le \infty$ and so, on justifying the limit at ∞,

$$\left(\int_0^\infty \exp(-t^2)\, dt \right)^2 \;=\; f(\infty) \;=\; g(0) \;=\; \arctan(1) \;=\; \frac{\pi}{4}.$$

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*

$$K(k) = \int_0^{\pi/2} \frac{1}{\sqrt{1 - k^2 \sin^2(s)}}\, ds$$

$$E(k) = \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2(s)}\, ds \tag{5.53}$$

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:

$$\frac{dK(k)}{dk} = \frac{E(k) - (1 - k^2)K(k)}{k(1 - k^2)} \qquad \frac{dE(k)}{dk} = \frac{E(k) - K(k)}{k}.$$

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

$$\lim_{t \to 0} f(t) = \frac{\pi}{2} + \lim_{t \to 0}(K(t) - E(t))K'(t) = \frac{\pi}{2}.$$

$\square$

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 [74].

In a similar manner, we next evaluate $K(1/\sqrt{2})$ and $E(1/\sqrt{2})$.

```
alias(K=EllipticK,E=EllipticE):k0:=1/sqrt(2);
K_0:=Int(1/sqrt(1-k0^2*sin(s)^2),s=0..Pi/2);
K1:=changevar(t=sin(s),K_0,t);assume(x>0,x<1):
K1:=simplify(changevar(x^2=t^2/(2-t^2),K1,x),symbolic);
K1:=simplify(changevar(u=x^4,K1,u));
```

The changes of variables $(s \to t \to x \to u)$ given in this *Maple* code reduces to

$$K\left(\frac{1}{\sqrt{2}}\right) \;=\; \frac{1}{2\sqrt{2}}\beta\left(\frac{1}{2},\frac{1}{4}\right) \;=\; \frac{\sqrt{\pi}\Gamma(\frac{1}{4})}{\sqrt{8}\Gamma(\frac{3}{4})} \;=\; \frac{\Gamma^2(\frac{1}{4})}{4\sqrt{\pi}},$$

on using (5.39), (5.40) and (5.42). By combining similar computations with (5.53), we may deduce that

$$E\left(\frac{1}{\sqrt{2}}\right) \;=\; \frac{4\Gamma^2(\frac{3}{4}) + \Gamma^2(\frac{1}{4})}{8\sqrt{\pi}}.$$

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

$$a_{n+1} \;=\; \frac{a_n + b_n}{2}, \qquad b_{n+1} \;=\; \sqrt{a_n b_n}. \tag{5.55}$$

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 [74]. 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

$$I(a,b) \quad = \quad I(A(a,b), G(a,b)), \tag{5.57}$$

where $A(a,b) = (a+b)/2$ and $G(a,b) = \sqrt{ab}$. Once this is shown, we have

$$I(a,b) \quad = \quad I(a_n, b_n) \quad = \quad \cdots \quad = \quad I(M(a,b), M(a,b)) \quad = \quad \frac{\pi/2}{M(a,b)},$$

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.

```
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, $j0/j$, simplifies as required. This is achieved by a *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)));
  resultant( p1,p2,R); simplify(series(j/j0,u,8));
```

and for peace of mind, the series of $j/j0$ can be computed! $\square$

Placing together (5.54) and (5.56), we have succeeded in establishing the discovery of Gauss in the form

$$M(\sqrt{2}, 1) = \sqrt{\frac{2}{\pi}} \, \Gamma^2 \left(\frac{3}{4} \right) = 1.198140234735592207439922492280323 8\ldots,$$

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.

5.6.3 Other Mean Iterations

Finally, the more general study of means [74] 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

$$a_{n+1} = M(a_n, b_n), \qquad b_{n+1} = N(a_n \, b_n)$$

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

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

While it is hard to guess the (linearly convergent) limit, once told that it is the *logarithmic mean*

$$\mathcal{L}(a, b) = \frac{a - b}{\log(a) - \log(b)},$$

proof of this fact reduces to showing the identity

$$\mathcal{L}(a, b) = \mathcal{L}\left(\frac{a + \sqrt{ab}}{2}, \frac{b + \sqrt{ab}}{2}\right). \qquad (5.58)$$

The following *Maple* code implements the iteration:

```
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;c;end;
```

Thus, a hundred iterates yields

$$L(2., 1., 100.) = 1.44269504088896340735992468100149976\ldots,$$

while

$$\mathcal{L}(2, 1) = 1.44269504088896340735992468100018921\ldots,$$

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

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

converges to

$$\mathcal{B}(a, b) = \frac{\sqrt{b^2 - a^2}}{\arccos(a/b)}$$

for $0 < a < b$, and to

$$\mathcal{B}(a, b) = \frac{\sqrt{a^2 - b^2}}{\text{arccosh}(a/b)}$$

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

$$\frac{\pi}{4} = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{2k - 1} \tag{5.59}$$

and

$$\frac{\pi^2}{6} = \sum_{k=1}^{\infty} \frac{1}{k^2}. \tag{5.60}$$

For the former, consider

$$\cot(x) = \frac{\cot(x/2) - \cot(\pi/2 - x/2)}{2} \tag{5.61}$$

and then observe that a telescoping identity yields

$$2^{-n} \sum_{k=1}^{2^n - 1} (-1)^k \cot\left(\frac{(2k+1)\frac{\pi}{4}}{2^n}\right) = 1.$$

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

$$\csc^2(x) \quad = \quad \frac{\csc^2(x/2) + \csc^2(\pi/2 + x/2)}{4}, \qquad (5.62)$$

and that a telescoping sum yields

$$2\,4^{-n} \sum_{k=1}^{2^{n-1}-1} \csc^2\left(\frac{(2k+1)\pi}{2^{n+1}}\right) \quad = \quad 1.$$

Again, taking limits carefully establishes

$$\frac{\pi^2}{8} \quad = \quad \sum_{k=1}^{\infty} \frac{1}{(2k-1)^2},$$

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 [157].]

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

$$\Gamma(x) = \frac{e^{-\gamma x}}{x} \prod_{n=1}^{\infty} \left[\frac{e^{x/n}}{1 + \frac{x}{n}} \right],$$

for $x > 0$. *Hint*: Use the definition of γ 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,

$$\int_{[0,1]^n} \frac{dx_1 \cdots dx_n}{(1 + x_1^2 + \cdots + x_n^2)^{(n+1)/2}} = \frac{\pi^{(n+1)/2}}{(n+1)2^n \Gamma(\frac{n+1}{2})}.$$

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 nth of the n-dimensional hypercube. So symmetry and setting $y_n = 1/x_n$, $y_j = x_j y_n$ for $1 \le j \le n-1$ gives

$$
\begin{aligned}
J &= n \int_0^\infty \int_{[0,y_n]^{n-1}} \frac{dy_1 \cdots dy_n}{(1 + y_1^2 + \cdots + y_n^2)^{(n+1)/2}} \\
&= n \int_0^\infty \int_{[0,1]^{n-1}} \frac{dx_1 \cdots dx_n}{(1 + x_1^2 + \cdots + x_n^2)^{(n+1)/2}} \\
&= n \int_0^1 \int_{[0,1]^{n-1}} \frac{dx_1 \cdots dx_n}{(1 + x_1^2 + \cdots + x_n^2)^{(n+1)/2}} \\
&\quad + n \int_1^\infty \int_{[0,1]^{n-1}} \frac{dx_1 \cdots dx_n}{(1 + x_1^2 + \cdots + x_n^2)^{(n+1)/2}} \\
&= nA + n \int_0^1 \int_{[0,y_n]^{n-1}} \frac{dy_1 \cdots dy_n}{(1 + y_1^2 + \cdots + y_n^2)^{(n+1)/2}} \\
&= (n+1)A.
\end{aligned}
$$

Thus

$$A = \frac{J}{n+1} = \frac{1}{(n+1)2^n} \int_{-\infty}^\infty \cdots \int_{-\infty}^\infty \frac{dy_1 \cdots dy_n}{(1 + y_1^2 + \cdots + y_n^2)^{(n+1)/2}}.$$

We may now apply a standard result for radially invariant integrals over 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 Ψ 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 $\Psi(n) = \sum_{k=1}^{n} 1/k - \gamma$. Obtain a similar formula for $\Psi(n + 1/2)$, for $n \in \mathrm{N}$.

(b) Prove that
$$\Psi(z) - \Psi(1 - z) = \pi \cot(\pi z).$$

(c) Obtain a duplication formula for Ψ from that of Γ.

(d) Show that
$$\Psi(z) = \int_0^{\infty} \frac{e^{-t} - e^{-zt}}{1 - e^{-t}} \, dt - \gamma$$
and that for $n = 1, 2, 3, \cdots$

$$\Psi^{(n)}(z) = (-1)^{n+1} \int_0^{\infty} \frac{t^n e^{-zt}}{1 - e^{-t}} \, dt$$

for $\mathrm{Re}\, z > 0$.

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 $\mathcal{E}$, 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 $\mathcal{E}$ is $(1-x)\mathcal{E}' = x\mathcal{E}$; 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

$$a(x) = \int_0^{\infty} \frac{e^{-t} \sin(xt)}{\sqrt{t}} dt \qquad\qquad (5.63)$$

$$b(x) = \int_0^{\infty} \frac{e^{-t} \cos(xt)}{\sqrt{t}} dt \qquad\qquad (5.64)$$

for $x > 0$ and so, or otherwise, solve for a and b explicitly. Answer:

$$\sqrt{\frac{\pi \left(\sqrt{1+x^2} \pm 1\right)}{2(1+x^2)}},$$

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

$$na_n = 2(a_{n-1} + a_{n-2}).$$

Show that the ordinary generating function satisfies $\mathcal{O}' = 2(1+x)\mathcal{O}$, and thus $\mathcal{O}(x) = \exp((1+x)^2)$. 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 $2^{n-1}(2^n - 1)$ such sequences. *Hint*: The number is

$$\sum_{\pi} \frac{1}{m_0! m_1! m_2! m_3!}$$

summed over all partitions of $n = m_0 + m_1 + m_2 + m_3$ with m_0 odd. The exponential generating function is $\mathcal{E}(x) = \sinh(x)(\exp(x))^3$.

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* $\text{Li}_3(x) = \sum_{n=1}^{\infty} x^n/n^3$. 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 [201, 6.3.3] gives as (6.13) the identity

$$\text{Li}_3\left(\frac{3-\sqrt{5}}{2}\right) = \frac{4}{5}\text{Li}_3(1) + \frac{\pi^2}{15}\log\left(\frac{3-\sqrt{5}}{2}\right) - \frac{1}{12}\log^3\left(\frac{3\sqrt{5}}{2}\right)$$

$$\tag{5.65}$$

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
>
> $$\frac{1}{1^3} + \frac{1}{2^3} + \frac{1}{3^3} + \cdots = \frac{\theta^2}{1^3} + \frac{\theta^4}{2^3} + \frac{\theta^6}{3^3} + \cdots, \quad \text{where} \quad \theta = 2\sin(\pi/10).$$
>
> 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 $\mathrm{Li}_3(1)$ and $\mathrm{Li}_3[(3-\sqrt{5})/2]$, if one should exist, would enable each to be isolated with the aid of (6.13), and there is no reason to expect that $\mathrm{Li}_3(1)$ 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^1 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^1 and (b) show that all eigenvalues are positive. *Hint*: Use *Maple* or *Mathematica* to find this determinant. Answer: (a) $\det(M_n^1) = n + 1$. (b) M_n^1 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.

19. **Berkeley problem 7.6.13.** Is there a real square matrix with $A^2 + 2A + 5I = 0$? *Hint*: Try some 2×2 examples. Answer: Yes.

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 cardiod in the complex plane. What can be found as a complex extension of $(a_1 + a_2 + \cdots + a_n)/n \geq (a_1 a_2 \cdots a_n)^{1/n}$ 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 [49].

(a) Consider the following analogue of Viéte's formula:

$$\mathcal{P} = \frac{\sqrt{2}}{\sqrt{1 + \sqrt{2}} \sqrt{1 + \frac{\sqrt{2}}{\sqrt{1 + \sqrt{2}}}} \sqrt{1 + \frac{\sqrt{2}}{\sqrt{1 + \frac{\sqrt{2}}{\sqrt{1 + \sqrt{2}}}}}}} \cdots .$$

By writing a recursion for $\mathcal{P}$, 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 $\left(1/\sqrt{2}\right)/4$.

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

$$\sum_{n=1}^{\infty} \frac{2^n \left[1 - \cos\left(x/2^n\right)\right]^2}{\sin\left(x/2^{n-1}\right)} = \tan\left(\frac{x}{2}\right) - \frac{x}{2}, \quad |x| < \pi$$

and

$$2\sum_{n=1}^{\infty} \frac{1 - \cos\left(x/2^n\right)}{\sin\left(x/2^{n-1}\right)} = \tan\left(\frac{x}{2}\right), \quad |x| < \pi.$$

These arose from dissecting a kite (recursively) into a circular sector and triangles [102].

25. **From Ramanujan's lost notebook.** The following examples appeared in Ramanujan's lost notebook [50]:

   (a) For $t \geq 0$ and $a > 0$, evaluate

$$\begin{aligned}
\mathcal{I}(a,t) &= \int_{-t}^{\infty} \frac{a^x}{\Gamma(x+1)} dx \\
&+ \int_0^{\infty} \frac{e^{-ax} x^{t-1}}{\pi^2 + \log^2(x)} \left(\cos(\pi t) - \frac{\sin(\pi t)}{\pi} \log(x)\right) dx.
\end{aligned}$$

   (b) Hence, for $s \geq 0$, evaluate

$$\mathcal{J}(s) = \int_0^{\infty} \frac{s^x}{\Gamma(x+1)} dx + \int_0^{\infty} \frac{e^{-sx}}{x\left(\pi^2 + \log^2(x)\right)} dx = \mathcal{I}(s,0).$$

   (c) For $t \geq 0$ and $a > 0$, evaluate

$$\begin{aligned}
\mathcal{K}(a,t) &= \int_{-t}^{\infty} \frac{a^x}{\Gamma(x+1)} dx \\
&+ \frac{\pi}{2} \int_0^{\infty} \left(\frac{e^{i\pi(t+ix)}}{a^{t+ix}} \Gamma(t+ix) + \frac{e^{-i\pi(t-ix)}}{a^{t-ix}} \Gamma(t-ix)\right) dx.
\end{aligned}$$

   (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 $\mathcal{I}$ with respect to t, show $\mathcal{I}(a,t)$ is a function of a alone. By differentiating $\mathcal{I}$ with respect to a, identify the function up to a multiplicative constant. Evaluate $\mathcal{I}(0,0)$ to obtain the constant.

(c) More elaborately, show $\mathcal{K}(t, a)$ satisfies the same differential equation and finally, identify the constant by showing $\mathcal{K}(1,0) = \mathcal{J}(1)$.

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.

6 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.

> – J. W. Tukey, "The Future of Data Analysis," *Annals of Mathematical Statistics*, 1962 [277]

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 [108, 109].

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

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

$$A_k(x, y) \quad = \quad \sum_{i+j=k} x_i y_j \qquad 0 \leq k < 2n. \tag{6.1}$$

The cyclic convolution of x and y is defined as n-long vector

$$C_k(x, y) \quad = \quad \sum_{i+j=k} x_i y_j \qquad 0 \leq k < n \tag{6.2}$$

$$= \quad \sum_{j=0}^{n-1} x_j y_{k-j}, \tag{6.3}$$

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:

$$F_k(z) \quad = \quad \sum_{j=0}^{n-1} z_j e^{-2\pi i j k/n} \qquad 0 \leq k < n$$

$$F_k^{-1}(z) \quad = \quad \frac{1}{n} \sum_{j=0}^{n-1} z_j e^{2\pi i j k/n} \qquad 0 \leq k < n. \tag{6.4}$$

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

$$A_k(x, y) \quad = \quad \sum_{j=0}^{2n-1} x_j x_{k-j}, \qquad 0 \le k < 2n, \qquad (6.5)$$

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

$$c_k \quad = \quad F_k^{-1}[F_j(a)F_j(b)], \qquad 0 \le k < 2n. \qquad (6.6)$$

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. 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 [14, 282].

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

$$\hat{f}(x) \quad = \quad \int_{-\infty}^{\infty} f(t)e^{-itx} \, dx \qquad (6.7)$$

(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

$$
\hat{f}\left(\frac{bk}{n}\right) \;=\; \int_{-\infty}^{\infty} f(t)e^{-itbk/n}\, dt
$$

$$
\approx \;\; \frac{a}{n} \sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} f\left(\frac{aj}{n}\right) e^{-i(aj/n)(bk/n)} \tag{6.8}
$$

$$
= \;\; \frac{a}{n} \sum_{j=-\frac{n}{2}+1}^{\frac{n}{2}+1} f\left(\frac{aj}{n}\right) e^{-2\pi ijk/n}, \tag{6.9}
$$

for $-n/2 + 1 \le k \le n/2$. 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

$$
\hat{f}\left(\frac{bk}{n}\right) \;=\; \frac{a}{n} \sum_{j=0}^{n-1} f\left(\frac{aj}{n}\right) e^{-2\pi ijk/n}, \tag{6.10}
$$

for $0 \le k \le n - 1$, 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 [118].

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 $10^{\pm 38}$. The IEEE "double" (64-bit) format features roughly 16 decimal digit accuracy and a dynamic range of $10^{\pm 308}$. 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.

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 $\oplus, \ominus$ and $\otimes$ 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 $a = a_{\mathrm{hi}} + a_{\mathrm{lo}}$.

1. $t := (2^{27} + 1) \otimes a$;
2. $a_{\mathrm{hi}} := t \ominus (t \ominus a)$;
3. $a_{\mathrm{lo}} := a \ominus a_{\mathrm{hi}}$;
4. Return $(a_{\mathrm{hi}}, a_{\mathrm{lo}})$.   □

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. $(a_{\mathrm{hi}}, a_{\mathrm{lo}}) := \mathrm{SPLIT}(a)$;
3. $(b_{\mathrm{hi}}, b_{\mathrm{lo}}) := \mathrm{SPLIT}(b)$;
4. $e := ((a_{\mathrm{hi}} \otimes b_{\mathrm{hi}} \ominus p) \oplus a_{\mathrm{hi}} \otimes b_{\mathrm{lo}} \oplus a_{\mathrm{lo}} \otimes b_{\mathrm{hi}}) \oplus a_{\mathrm{lo}} \otimes b_{\mathrm{lo}}$;
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 $e := a \otimes b - p$. 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 [170].

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

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 $10^{\pm 308}$ 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 $\pm$ 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

$$A = \pm(2^{pb}m_1 + 2^{(p-1)b}m_2 + 2^{(p-2)b}m_3 + \cdots + 2^{(p-n+1)b}m_n),$$

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 [38]. 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.

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.

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 [182]. 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 [118]:

$$t = (x_0 + x_1) \cdot (y_0 + y_1) \tag{6.11}$$

$$u = (x_0 - x_1) \cdot (y_0 - y_1) \tag{6.12}$$

$$v = x_1 y_1 \tag{6.13}$$

$$xy = \frac{1}{2}(t + u) - v + \frac{B}{2}(t - u) + vB^2 \tag{6.14}$$

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-

duced 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 [118].

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 π, 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:

$$c_k \quad = \quad \sum_{j=0}^{2n-1} a_j b_{k-j}, \qquad 0 \le k < 2n, \qquad (6.15)$$

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:

$$
\begin{aligned}
z_0 &= x_0 y_0 + x_{p-1} y_{p+1} + x_p y_p + x_{p+1} y_{p-1} \\
z_1 &= x_0 y_1 + x_1 y_0 + x_p y_{p+1} + x_{p+1} y_p
\end{aligned}
$$

$$
\begin{aligned}
z_2 &= x_0 y_2 + x_1 y_1 + x_2 y_0 + x_{p+1} y_{p+1} \\
z_3 &= x_0 y_3 + x_1 y_2 + x_2 y_1 + x_3 y_0 \\
\cdots &= \cdots \\
z_p &= x_0 y_p + x_1 y_{p-1} + \cdots + x_p y_0 \\
\cdots &= \cdots \\
z_{2p-1} &= x_{p-2} y_{p+1} + x_{p-1} y_p + x_p y_{p-1} + x_{p+1} y_{p-2} \quad (6.16)
\end{aligned}
$$

This result differs from the desired $2n$-long linear convolution of x and y in two respects: (1) the initial three values (z_0, z_1 and z_2) are "corrupted" with some additional terms, and (2) the final four members of the sequence are missing. These four missing values are

$$
\begin{aligned}
z_{2n-4} &= z_{2p} = x_{p-1} y_{p+1} + x_p y_p + x_{p+1} y_{p-1} \\
z_{2n-3} &= z_{2p+1} = x_p y_{p+1} + x_{p+1} y_p \\
z_{2n-2} &= z_{2p+2} = x_{p+1} y_{p+1} \\
z_{2n-1} &= z_{2p+3} = 0 \quad (6.17)
\end{aligned}
$$

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 [17, 119].

Additional results and techniques for using various types of FFTs for high-precision arithmetic can be found in Crandall's books on mathematical computation [119, 118].

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
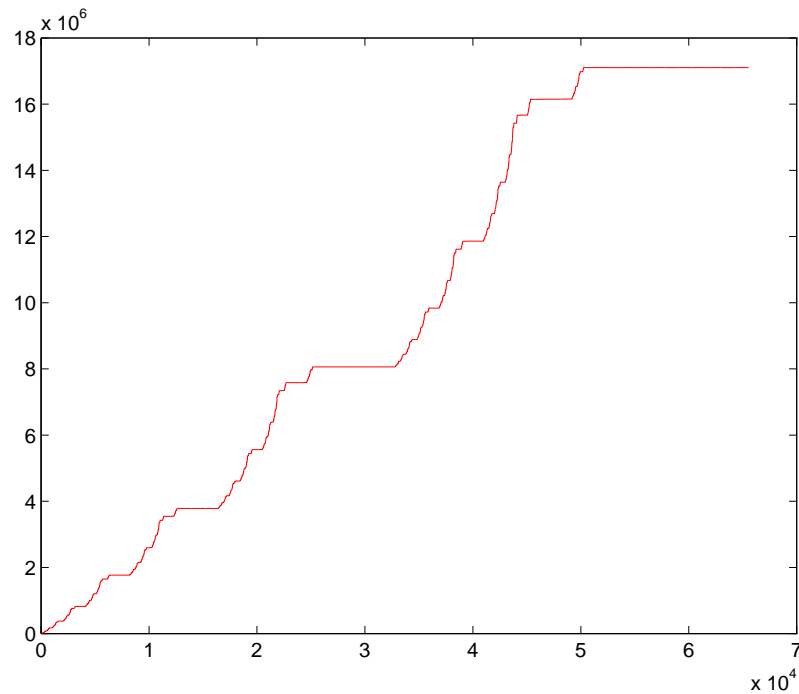
Figure 6.1. Computational cost for the devil's convolution.

here only an informal sketch of these methods. See [15, 38] for additional details.

We start with a scheme for extra-high precision division. As we mentioned earlier, for moderate precision levels an adaptation of the conventional 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:

$$x_{k+1} \quad = \quad x_k + x_k(1 - bx_k). \tag{6.18}$$

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 $1/\sqrt{a}$:

$$x_{k+1} \quad = \quad x_k + \frac{x_k}{2}(1 - ax_k^2). \tag{6.19}$$

Multiplying the final approximation to $1/\sqrt{a}$ by a gives the square root of a. Some additional details are given in [38].

Algorithm 6.55. *Pi.*

The constant π, 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 $k = 1$:

$$\begin{aligned}
a_k &= (a_{k-1} + b_{k-1})/2 \\
b_k &= \sqrt{a_{k-1}b_{k-1}} \\
d_k &= d_{k-1} - 2^k(a_k - b_k)^2.
\end{aligned} \tag{6.20}$$

Then $p_k = (a_k + b_k)^2/d_k$ converges quadratically to π—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 π 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:

$$e^t \quad = \quad \left(1 + r + \frac{r^2}{2!} + \frac{r^3}{3!} + \frac{r^4}{4!} \cdots\right)^{256} 2^n, \tag{6.21}$$

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

$$x_{k+1} \quad = \quad x_k + \frac{a - e^x}{e^x}, \tag{6.22}$$

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 [86]. 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:

$$\log 2 \quad = \quad \frac{\pi}{2mA(1, 4/2^m)}. \tag{6.23}$$

Here $A(a, b)$ is the limit of the AGM: Let $a_0 = a$ and $b_0 = b$, and iterate

$$a_{k+1} \quad = \quad (a_k + b_k)/2 \qquad b_{k+1} \quad = \quad \sqrt{a_k b_k} \tag{6.24}$$

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:

$$\log t \quad = \quad \frac{\pi}{2A(1, 4/s)} - m\log 2. \tag{6.25}$$

Given this scheme for logarithms, very high-precision exponentials can be calculated using Newton iterations, using a doubling level of precision as before.

Algorithm 6.59. *Sin and cos.*

For modest precision, one can calculate $\sin t$ via the Taylor's series

$$\sin s \;=\; s - \frac{s^3}{3!} + \frac{s^5}{5!} - \frac{s^7}{7!} \cdots , \qquad (6.26)$$

where $s = t - a\pi/256$, and where the integer a is chosen to minimize the absolute value of s. Then one calculates

$$\begin{aligned}
\sin t &= \sin(s + a\pi/256) \\
\cos t &= \cos(s + a\pi/256),
\end{aligned}$$

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 [38] 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.

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

$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n = 0$. 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 [140].

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 [163], 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 [139], which was discovered in 1993 by Helaman Ferguson. PSLQ originally came to prominence with its role in the discovery of the BBP formula for π. 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 [139, 18, 35], 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 $H_{ij} := -y_i y_j/(s_j s_{j+1})$ 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 $m \le n - 2$ 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 $j := \min(i - 1, m + 1)$ 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 [35].

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 $H_{ij} := -y_i y_j/(s_j s_{j+1})$; 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 βn 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 $t_0 := \sqrt{H_{m_i,m_i}^2 + H_{m_i,m_i+1}^2}$, $t_1 := H_{m_i,m_i}/t_0$ and $t_2 := H_{m_i,m_i+1}/t_0$; for $i := m_i$ to n do: set $t_3 := H_{i,m_i}$; $t_4 := H_{i,m_i+1}$; $H_{i,m_i} := t_1 t_3 + t_2 t_4$; and $H_{i,m_i+1} := -t_2 t_3 + t_1 t_4$; 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 $H_{lj} := H_{lj} - T_{lk}H_{kj}$; enddo; set $T_{lj} := \text{nint}(H_{lj}/H_{jj})$ and $H_{lj} := H_{lj} - T_{lj}H_{jj}$; 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. $\square$

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 βn 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 βn disjoint pairs of indices in Step 2 above has the effect of reducing the iteration count by nearly the factor βn. 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 multi-pair PSLQ algorithm appears to be significantly faster than the standard PSLQ [35]. 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.

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 α is the input numerical constant) [40].

1. Table look-up. An indexed table of well-known numerical constants is checked to see if it contains α, 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 α 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 π, e, $\log 2$, $\log 3$, G and γ (here G is Catalan's constant and γ is Euler's gamma constant). If a relation is found in this set of numbers, then this means α is given by a one-term formula of the form

$$\alpha = \pm 2^a 3^b 5^c 7^d 11^e 13^f 17^g 19^h \pi^k e^l (\log 2)^m (\log 3)^n G^o \gamma^p$$

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://ddrive.cs.dal.ca/~isc/. Software that performs this type of search strategy is also available as part of the Experimental Mathematician's Toolkit: http://www.experimentalmath.info. Another interesting resource in this regard is Finch's recently published *Mathematical Constants* [141].

Maple 9, released in summer 2003, incorporates a quite functional constant recognition tool. Typing `identify(3.146264370)` returns $3^{1/2} + 2^{1/2}$. 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 π 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 $\{a_i\}$ be the continued fraction expansion of a random real number. The *Gauss-Kuz'min distribution* states that

$$\mathrm{Prob}(a_n = k) \;=\; -\log_2 \left[1 - \frac{1}{(k+1)^2} \right].$$

Khintchine showed that, $\lim_k (a_1 a_2 \cdots a_k)^{1/k}$, the limiting geometric

mean, exists a.e. and equals

$$K_0 = \prod_{k=1}^{\infty} \left[1 + \frac{1}{k(k+2)} \right]^{\log_2 k} = \prod_{k=1}^{\infty} k^{\left[\log_2 \left(1 + \frac{1}{k(k+2)} \right) \right]}$$

$$= 2.6854520010653064453097148354817956938203822939 9446 \dots$$

Little is known about K_0. Is it rational, algebraic, or related to π or e? The formula is very slowly convergent.

For any positive integer N, we may, however, derive a quite effective identity

$$\log(K_0) \log(2) \quad = \quad \sum_{s=1}^{\infty} \zeta(2s, N) \frac{A_s}{s} - \sum_{k=2}^{N} \log \left(1 - \frac{1}{k} \right) \log \left(1 + \frac{1}{k} \right),$$

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 [26].

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

$$10^{1000} \sqrt{N} = \frac{\sqrt{10^{3998} - 10^{2000}}}{3},$$

and so

$$\frac{10^{1999} - 6}{3} < 10^{1000} \sqrt{N} < \frac{10^{1999} - 4}{3}.$$

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 [77]. 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

$$\frac{dy}{dt} = y^2, \tag{6.27}$$

with $y(0) = y_0$? The numerical procedure is just

$$y_{n+1} = y_n + hy'_n \tag{6.28}$$

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

$$\frac{dv}{d\tau} = v^2, \tag{6.29}$$

and (6.28) becomes

$$v_{n+1} = v_n + v_n^2. \tag{6.30}$$

We may then rephrase our question to ask instead what the relationship between v_n and $v(\tau)$ is.

The point of view taken in [111] 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

$$\frac{dw}{d\tau} = B(w)w^2, \tag{6.31}$$

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* [156] 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

$$\frac{dw}{dt} = \left(1 - w + \frac{3}{2!}w^2 - \frac{16}{3!}w^3 + \frac{124}{4!}w^4 - \frac{1256}{5!}w^5\right)w^2. \tag{6.32}$$

Now we see the sequence $1, -1, 3, -16, 124, -1256$ appearing. This is sequence M3024 in Sloane's dictionary [262], which points us directly to the very beautiful and useful paper [196]. It tells us that if

$$B(w) = \sum_{n \geq 0} c_n w^n, \tag{6.33}$$

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 $v \to v + v^2$ 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 [111] for details.
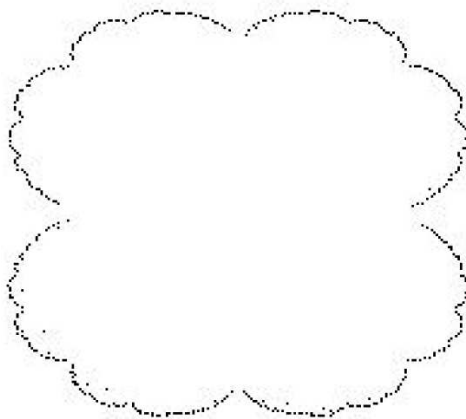
Figure 6.2. The first 16,000 poles of $B(v)$, approaching the Julia set of $v \to v + v^2$.

5. **Accelerations for Catalan's constant.** (This material is condensed from [85].) 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

$$G \;=\; \frac{\pi}{8}\log(2+\sqrt{3}) + \frac{3}{8}\sum_{k=0}^{\infty}\frac{1}{(2k+1)^2\binom{2k}{k}}, \qquad (6.34)$$

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 π times the logarithm of an algebraic unit (i.e., an invertible algebraic integer). The most striking example is

$$G \;=\; \frac{\pi}{8}\log\left(\frac{10+\sqrt{50-22\sqrt{5}}}{10-\sqrt{50-22\sqrt{5}}}\right) + \frac{5}{8}\sum_{k=0}^{\infty}\frac{L_{2k+1}}{(2k+1)^2\binom{2k}{k}}, \qquad (6.35)$$

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

$$G \;=\; -\int_0^{\pi/4}\log(\tan\theta)\,d\theta, \qquad (6.36)$$

obtained by expanding the integrand into its Fourier cosine series and integrating term by term. Ramanujan's result (6.34) arises from the transformation

$$2\int_0^{\pi/4}\log(\tan\theta)\,d\theta \;=\; 3\int_0^{\pi/12}\log(\tan\theta)\,d\theta. \qquad (6.37)$$

Formula (6.35) arises similarly from the transformation

$$2\int_0^{\pi/4}\log(\tan\theta)\,d\theta$$
$$= 5\int_0^{3\pi/20}\log(\tan\theta)\,d\theta - 5\int_0^{\pi/20}\log(\tan\theta)\,d\theta. \qquad (6.38)$$

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, 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
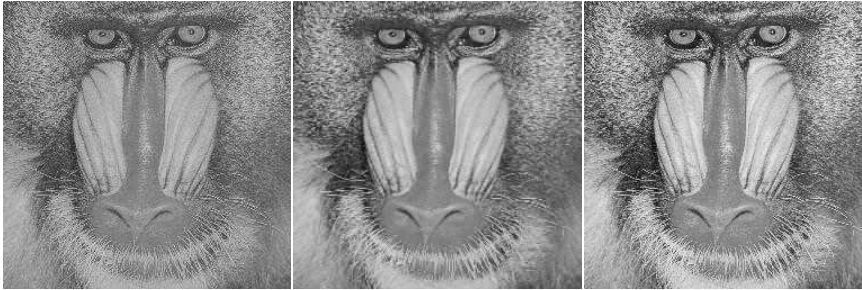
Figure 6.3. Three images quantized at quality 50 (L), 48 (C) and 75 (R). Courtesy of Mason Macklem.

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 ([45] and [209]). 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 [123]. 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 *if* acquires when written $\supset$, a virtue it did not possess when written if."

   (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 [123] 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 | Recent Experiences

We [Kaplansky and Halmos] share a philosophy about linear algebra:
we think basis-free, we write basis-free, but when the chips are down
we close the office door and compute with matrices like fury.

> – Irving Kaplansky, 1917–2006. Quoted in Paul Halmos' *Celebrating 50 Years of Mathematics*.

We take the opportunity in this chapter to describe three pieces of experimental mathematics and related research that have been performed since our earlier publications [72, 25] and the earlier edition of this book [71]. In addition, from discussions with colleagues and lectures to various groups, our own thoughts have been refined and revised. In consequence, we have added some more discursive sections as bookends. We have also aggregated a mélange of examples and exercises—some generated by the sections and some totally unrelated.

7.1   Doing What Is Easy

We start this chapter with a section that re-explores "easy" tools available in almost any symbolic computation system—or other high-level language—and their powerful consequences. The theme of this section might well be "It's a computer, stupid!" So let us recall some of the things computers do better than humans. These include

1. High precision arithmetic—the mathematical electron microscope (Sections 7.1, 7.4, and 7.5);

2. Formal power-series manipulation, e.g., summing squares and cubes (Sections 7.1, 7.2, and Exercise 33);

3. Changing representations, e.g., continued fraction expansions (Section 7.1, Exercises 20, and 21);

4. Changing representations, e.g., partial fractions expansions (Exercises 16, 23, and 33);

5. Changing representations, e.g., Padé approximations (Section 7.1, Exercises 20, 21, and 22);

6. Recursion solving, e.g., by using Rsolve in *Mathematica* or rsolve and gfun in *Maple* (Section 7.1, 7.2, Exercises 9, and 44);

7. Integer relation algorithms, e.g. by using identify and MinimalPolynomial (or minpoly) in *Maple* or RootApproximant in *Mathematica* (Section 7.1, 7.3, Exercises 9, and 42);

8. Creative telescoping, e.g., the Gosper and Wilf-Zeilberger methods (Section 7.1, 7.2, and Exercise 9);

9. Pictures, pictures, pictures: intuition, simulation and more (Exercises 24, 29, and 31).

All of these have been described in this volume and others [71, 25], and all bear re-examination. The parenthetic numbers above refer to exemplary sections or exercises in this chapter that explore the given topic. Before we launch into the matter, we repeat some mantras.

- Always be suspicious; try to numerically confirm any symbolic discovery.

- As in any other experimental subject, one cannot prove anything. One can, however, be led to a proof (human or computer generated).

- Moreover, one can "falsify" (which in Karl Popper's accounting is central to the scientific method); but even negative results should be replicated.

We should add that most of the topics of the first two sections of this chapter are also well covered in a new book by Villegas [283] , which works in PARI/GP.

7.1.1   Hunting a Rational Sequence

For reasons that will be explained in Section 7.1.4, suppose we wish to determine a closed form for the sequence that starts with the following dozen terms:

$$1, -\frac{1}{3}, \frac{1}{25}, -\frac{1}{147}, \frac{1}{1089}, -\frac{3}{20449}, \frac{1}{48841}, -\frac{1}{312987}, \frac{25}{55190041},$$
$$-\frac{1}{14322675}, \frac{1}{100100025}, -\frac{49}{32065374675}.$$

We can easily supply at least 20 more values, the next six being

$$\frac{1}{4546130625}, -\frac{1}{29873533563}, \frac{9}{1859904071089}, -\frac{3}{4089135109921},$$
$$\frac{1}{9399479144449}, -\frac{363}{22568149425822049}.$$

What should we do?

- *Factorization* often helps. In this case, the first eight values after the initial 1 yield

$$\frac{-1}{(3)}, \frac{1}{(5)^2}, \frac{-1}{(3)(7)^2}, \frac{1}{(3)^2(11)^2}, \frac{(-3)}{(11)^2(13)^2}, \frac{1}{(13)^2(17)^2},$$
$$\frac{-1}{(3)(17)^2(19)^2}, \frac{(5)^2}{(17)^2(19)^2(23)^2}.$$

- The alternating signs and the signal role of 3 suggest separating the even and odd cases and taking square roots. The even terms then start

$$1, \frac{1}{(5)}, \frac{1}{(3)(11)}, \frac{1}{(13)(17)}, \frac{(5)}{(17)(19)(23)}, \frac{1}{(3)(5)(23)(29)},$$
$$\frac{1}{(3)(5)^2(29)(31)}, \frac{(3)}{(29)(31)(37)(41)}, \ldots.$$

After multiplication by -3 and taking square roots, the odd terms start

$$1, \frac{1}{(7)}, \frac{(3)}{(11)(13)}, \frac{1}{(17)(19)}, \frac{1}{(5)(19)(23)}, \frac{(7)}{(5)(23)(29)(31)},$$
$$\frac{1}{(3)(29)(31)(37)}, \frac{(3)}{(31)(37)(41)(43)}, \ldots.$$

- It is now apparent that both sequences have structure modulo 6. Indeed the largest value is of the form $6n \mp 1$ except in the even case of 35 and the odd case of 25, which are not prime. Were the modular pattern not so clear, we could have produced more cases and "reshaped" as in the next section.

- The engagement of $(6n \pm 1)!$ is now highly likely. Consider the even terms. When we multiply by $(6n)!$ we rapidly get enormous integers. If we try multiplying by the central binomial coefficient $\binom{6n}{3n}$, we obtain $\iota := 1, 4, 28, 220, 1820, 15504, 134596, 1184040, \ldots$. Entering this

into Sloane's Encyclopedia (which will be illustrated in some detail in Section 7.1.3) uniquely returns sequence A005810 and the closed form $\binom{4n}{n}$—or we might proceed as above with ι. Thus the even terms of our original sequence appear to satisfy $s_{2n} = \left(\binom{4n}{n}/\binom{6n}{3n}\right)^2$ with many alternate expressions. The odd terms are likewise discoverable; see Exercise 2.

We return to this discovery and its proof in Section 7.1.4.

7.1.2   Sums of Squares, Cubes, and So On

The ability to rapidly compute fundamental generating functions for quantities such as sums of squares [72, Chapter 4] is a tremendous source of insight for both research or pedagogical reasons. For example, the Jacobian theta function

$$\theta_3(q) \quad = \quad 1 + 2\sum_{n=1}^{\infty} q^{n^2}$$

is easy to manipulate symbolically or numerically. It is immediate that for $N = 2, 3, 4 \ldots$,

$$\theta_3^N(q) \quad = \quad 1 + \sum_{n=1}^{\infty} r_N(n)q^n,$$

where $r_N(n)$ counts the number of representations of n as a sum of N squares, counting sign and order. Let us examine the first three cases.

First, recall that if $P_a := \sum_{n=0}^{\infty} q^{a_n}$ is the generating function for a sequence $a = \{a_n\}$, then $P_a(q)P_b(q)$ counts the representations of numbers of the form $n = a_j + b_k$:

Sums of two squares

The ordinary generating function to order 49 is

$$\begin{aligned}
\theta_3^2(q) \quad = \quad & 1 + 4\,q + 4\,q^2 + 4\,q^4 + 8\,q^5 + 4\,q^8 + 4\,q^9 + 8\,q^{10} + 8\,q^{13} + 4\,q^{16} \\
& + 8\,q^{17} + 4\,q^{18} + 8\,q^{20} + 12\,q^{25} + 8\,q^{26} + 8\,q^{29} + 4\,q^{32} + 8\,q^{34} \\
& + 4\,q^{36} + 8\,q^{37} + 8\,q^{40} + 8\,q^{41} + 8\,q^{45} + \cdots, \quad\quad\quad (7.1)
\end{aligned}$$

from which it quickly becomes apparent that numbers of the form $4m + 3$ are missing and that $r_2(2n) = r_2(n)$. Both *Maple* and *Mathematica* have implementations of the θ-functions, and $\theta_3(q)$ implemented directly is

lacunary, so we could equally well have generated several hundred or even several thousand terms. In particular, we should quickly observe Fermat's result that an odd prime p is representable as a sum of two squares if and only if it is of the form $p = 4m + 1$. As discussed elsewhere [72, Chapter 4], the actual number of representations is $r_2(n) = 4(d_1(n) - d_3(n))$, where d_k counts the number of divisors congruent to k modulo four.

Sums of three squares

The ordinary generating function to order 49 is now

$$
\begin{aligned}
\theta_3^3(q) \;=\; & 1 + 6\,q + 12\,q^2 + 8\,q^3 + 6\,q^4 + 24\,q^5 + 24\,q^6 + 12\,q^8 + 30\,q^9 + 24\,q^{10} \\
& + 24\,q^{11} + 8\,q^{12} + 24\,q^{13} + 48\,q^{14} + 6\,q^{16} + 48\,q^{17} + 36\,q^{18} + 24\,q^{19} \\
& + 24\,q^{20} + 48\,q^{21} + 24\,q^{22} + 24\,q^{24} + 30\,q^{25} + 72\,q^{26} + 32\,q^{27} \\
& + 72\,q^{29} + 48\,q^{30} + 12\,q^{32} + 48\,q^{33} + 48\,q^{34} + 48\,q^{35} + 30\,q^{36} \\
& + 24\,q^{37} + 72\,q^{38} + 24\,q^{40} + 96\,q^{41} + 48\,q^{42} + 24\,q^{43} + 24\,q^{44} \\
& + 72\,q^{45} + 48\,q^{46} + 8\,q^{48} + 54\,q^{49} + O\left(q^{50}\right). \qquad\qquad (7.2)
\end{aligned}
$$

One thing is immediately clear: Most but not all numbers are a sum of three squares. This is easier to see if we look at the coefficients as a list:

$$
\begin{aligned}
& [6, 12, 8, 6, 24, 24, 0, 12, 30, 24, 24, 8, 24, 48, 0, 6, 48, 36, 24, 24, 48, 24, 0, 24, 30, \\
& \; 72, 32, 0, 72, 48, 0, 12, 48, 48, 48, 30, 24, 72, 0, 24, 96, 48, 24, 24, 72, 48, 0, 8, 54].
\end{aligned}
$$

Much more becomes apparent if we reshape the list into a matrix of appropriate dimensions. The *Maple* instruction

```
reshape:=(m,n,L)-> linalg[matrix](m,n,[seq(L[k],k=1..m*n)]);
```

will do this for a list L with at least $m \times n$ members. For example, a 7×7 reshaping of the first 49 elements produces

$$
\begin{bmatrix}
6 & 12 & 8 & 6 & 24 & 24 & 0 \\
12 & 30 & 24 & 24 & 8 & 24 & 48 \\
0 & 6 & 48 & 36 & 24 & 24 & 48 \\
24 & 0 & 24 & 30 & 72 & 32 & 0 \\
72 & 48 & 0 & 12 & 48 & 48 & 48 \\
30 & 24 & 72 & 0 & 24 & 96 & 48 \\
24 & 24 & 72 & 48 & 0 & 8 & 54
\end{bmatrix},
$$

whereas a 6×8 reshaping provides

$$
\begin{bmatrix}
6 & 12 & 8 & 6 & 24 & 24 & 0 & 12 \\
30 & 24 & 24 & 8 & 24 & 48 & 0 & 6 \\
48 & 36 & 24 & 24 & 48 & 24 & 0 & 24 \\
30 & 72 & 32 & 0 & 72 & 48 & 0 & 12 \\
48 & 48 & 48 & 30 & 24 & 72 & 0 & 24 \\
96 & 48 & 24 & 24 & 72 & 48 & 0 & 8
\end{bmatrix},
$$

and we see that no number of the form $8m + 7$ is a sum of three squares. The "rogue" zero is in the 28th place and is a first hint that the general result is that $r_3(n) = 0$ exactly for numbers of the form $4^k(8m + 7)$. The exact form of $r_3(n)$ is quite complex.

Sums of four squares

A similar process of reshaping the coefficients of the first 96 values of $r_4(n)/8$ produces

$$
\begin{bmatrix}
1 & 3 & 4 & 3 & 6 & 12 & 8 & 3 \\
13 & 18 & 12 & 12 & 14 & 24 & 24 & 3 \\
18 & 39 & 20 & 18 & 32 & 36 & 24 & 12 \\
31 & 42 & 40 & 24 & 30 & 72 & 32 & 3 \\
48 & 54 & 48 & 39 & 38 & 60 & 56 & 18 \\
42 & 96 & 44 & 36 & 78 & 72 & 48 & 12 \\
57 & 93 & 72 & 42 & 54 & 120 & 72 & 24 \\
80 & 90 & 60 & 72 & 62 & 96 & 104 & 3 \\
84 & 144 & 68 & 54 & 96 & 144 & 72 & 39 \\
74 & 114 & 124 & 60 & 96 & 168 & 80 & 18 \\
121 & 126 & 84 & 96 & 108 & 132 & 120 & 36 \\
90 & 234 & 112 & 72 & 128 & 144 & 120 & 12
\end{bmatrix}.
$$

This strongly suggests Lagrange's famous *four squares theorem* that every integer is the sum of four squares, for example, $7 = 4 + 1 + 1 + 1$ (see also Exercise 17). The exact form is also a divisor function [72, Chapter 4].

In general, a simple reshaping function is a remarkably useful tool for unearthing modular patterns in sequences; see also Exercise 49.

7.1.3   Hunting an integer sequence

Given an integer sequence, one should always recall the existence of Sloane's *On-Line Encyclopedia of Integer Sequences* (herein called Sloane's Encyclopedia). The *MathPortal* website at `http://ddrive.cs.dal.ca/~isc/portal` collects this tool as well as others in one place.

Suppose we are presented with

$$1, 1, 4, 9, 25, 64, 169, 441, 1156, 3025,$$

which you may well recognize right away. But whether you do or not, let us see what happens.

Using Sloane's Encyclopedia

Figure 7.1.3 illustrates the richness of the information available in Sloane's Encyclopedia. Indeed, $1, 1, 4, 9, 25, 64, 169$ suffices to identify the sequence uniquely among the roughly 133,000 sequences in the data base. The references, formulas, and recursions are substantial and reliable. The link to P. Stanica, for example, leads to a detailed paper on the *ArXiv*. Further on, there often is code in one or more packages. This time it is:

```
(PARI)   a(n)=fibonacci(n)^2
```

The most satisfactory strategy, if one has access to many terms of a sequence, is to use only as many terms as are necessary to produce a very few matches (ideally one) and then to experimentally confirm by matching your remaining terms to those listed in the database. For example, consider

$$1, 2, 4, 16, 31, 61, 120, 236, 464.$$

The terms up to 31 provided 22 matches, adding 61 reduced this to four, and adding 120 uniquely returns the *Pentanacci numbers*: $a(n + 1) = a(n) + ... + a(n - 4)$, which also agrees with the remaining terms and is preceded by a number of zeros and ones. Had we instead entered the sequence

$$1, 2, 4, 8, 16, 31, 61, 119, 232, 453,$$

the same process would recover "the number of compositions of n with parts in N which avoid the pattern 123," preceded by another number of zeros and ones. (As with the Fibonacci numbers it is not always clear how

Greetings from [The On-Line Encyclopedia of Integer Sequences](#)!

```
1,4,9,25,64,169,441,1156,3025
```
   Search

Hints

Search: **1, 4, 9, 25, 64, 169, 441, 1156, 3025**
Displaying 1-1 of 1 results found.   pag
  Format: long | short | internal | text   Sort: relevance | references | number   Highlight: on | off
A007598   F(n)^2, where F() = Fibonacci numbers A000045.
                (Formerly M3364)
   0, 1, **1, 4, 9, 25, 64, 169, 441, 1156, 3025**, 7921, 20736, 54289, 142129, 372100,
   974169, 2550409, 6677056, 17480761, 45765225, 119814916, 313679521, 821223649,
   2149991424, 5628750625, 14736260449, 38580030724 (list; graph; listen)

OFFSET	0,4
COMMENT	a(n)*(-1)^(n+1) = (2*(1-T(n,-3/2))/5), n>=0, with Chebyshev's polynomials T(n,x) of the first kind, is the r=-1 member of the r-family of sequences S_r(n) defined in A092184 where more information can be found. W. Lang (wolfdieter.lang_AT_physik_DOT_uni-karlsruhe_DOT_de), Oct 18 2004
REFERENCES	A. T. Benjamin and J. J. Quinn, Proofs that really count: the art of combinatorial proof, M.A.A. 2003, id. 8. R. Honsberger, Mathematical Gems III, M.A.A., 1985, p. 130. R. P. Stanley, Enumerative Combinatorics I, Example 4.7.14, p. 251.
LINKS	D. Foata and G.-N. Han, Nombres de Fibonacci et polynomes orthogonaux, T. Mansour, A note on sum of k-th power of Horadam's sequence T. Mansour, Squaring the terms of an ell-th order linear recurrence P. Stanica, Generating functions, weighted and non-weighted sums of powers...
FORMULA	a(0) = 0, a(1) = 1; a(n) = a(n-1) + Sum(a(n-i)) + k, 0 <= i < n where k = 1 when n is odd, or k = -1 when n is even. E.g. a(2) = 1 = 1 + (1 + 1 + 0) - 1, a(3) = 4 = 1 + (1 + 1 + 0) + 1, a(4) = 9 = 4 + (4 + 1 + 1 + 0) - 1, a(5) = 25 = 9 + (9 + 4 + 1 + 1 + 0) + 1. - Sadrul Habib Chowdhury (adil040(AT)yahoo.com), Mar 02 2004 G.f.: x(1-x)/((1+x)(1-3x+x^2)). a(n)=2a(n-1)+2a(n-2)-a(n-3), n>2. a(0)=0, a(1)=1, a(2)=1. a(-n)=a(n). (1/5)[2*Fibonacci(2n+1) - Fibonacci(2n) - 2(-1)^n]. - R. Stephan, May 14 2004 a(n) = F(n-1)F(n+1) - (-1)^n = A059929(n-1) - A033999(n). a(n) = right term of M^n * [1 0 0] where M = the 3X3 matrix [1 2 1 / 1 1 0 / 1 0 0]. M^n * [1 0 0] = [a(n+1) A001654(n) a(n)]. E.g. a(4) = 9 since M^4 * [1 0 0] = [25 15 9] = [a(5) A001654(4) a(4)]. - Gary W. Adamson (qntmpkt(AT)yahoo.com), Dec 19 2004 Sum_(j=0..2n) binomial(2n,j) a(j)= 5^(n-1) A005248(n+1) for n>=1 [P. Stanica]. sum_(j=0..2n+1) binomial(2n+1,j) a(j)=5^n A001519(n+1) [P. Stanica]. - Richard J. Mathar (mathar(AT)strw.leidenuniv.nl), Oct 16 2006

Figure 7.1. A sample of Sloane's information on $1, 1, 4, 9, 25, 64, 169, \ldots$.

a sequence is indexed.) Of course, even when not uniquely isolated, our research will often prefer one answer over another depending on how it arose in our work.

In a computer algebra package

Alternatively, the following sample *Maple* session, after loading the gfun package, illustrates that—in a very few lines—we can start with the sequence, guess its generating function, find its predicted recursion, explicitly develop its closed form and confirm the pattern with a few more terms.

```
>   s:=[seq(fibonacci(n)^2,n=1..10)];
```

$$s := [1,\ 1,\ 4,\ 9,\ 25,\ 64,\ 169,\ 441,\ 1156,\ 3025]$$

```
>   g:=guessgf(s,x)[1];
```

$$g := -\frac{1-x}{2\,x^2 - 1 + 2\,x - x^3}$$

```
>   r:=listtorec(s,u(n))[1];
```

$$r := \{-u(n+3) + 2\,u(n+2) + 2\,u(n+1) - u(n),\ u(0) = 1,\ u(1) = 1,\ u(2) = 4\}$$

```
>   r:=rsolve(%,u(n));
```

$$r := \frac{2\,(-1)^n}{5} - \frac{2\left(\dfrac{3}{2} - \dfrac{\sqrt{5}}{2}\right)^n\left(-\dfrac{3}{4} + \dfrac{\sqrt{5}}{4}\right)}{5} - \frac{2\left(\dfrac{3}{2} + \dfrac{\sqrt{5}}{2}\right)^n\left(-\dfrac{3}{4} - \dfrac{\sqrt{5}}{4}\right)}{5}$$

```
>   seq(expand(r(n)),n=1..13);
```

$$1,\ 4,\ 9,\ 25,\ 64,\ 169,\ 441,\ 1156,\ 3025,\ 7921,\ 20736,\ 54289,\ 142129$$

```
>   [seq(fibonacci(n)^2,n=2..14)];
```

$$[1,\ 4,\ 9,\ 25,\ 64,\ 169,\ 441,\ 1156,\ 3025,\ 7921,\ 20736,\ 54289,\ 142129]$$

7.1.4   Some Generalized Hypergeometric Values

A hypergeometric evaluation

In our book *Experimental Mathematics in Action*, we described the discovery and proof of a generating function for the even ζ-values [25, Section 3.6]. The discovery relied heavily both on integer detection methods and on

computing Padé approximants. The general result that we found is given
as Theorem 7.0.

Theorem 7.63. *Let x be a complex number not equal to a nonzero integer.*
Then

$$\sum_{k=1}^{\infty} \frac{1}{k^2 - x^2} \quad = \quad 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k} \left(1 - \frac{x^2}{k^2}\right)} \prod_{m=1}^{k-1} \left(\frac{1 - \frac{4x^2}{m^2}}{1 - \frac{x^2}{m^2}} \right). \qquad (7.3)$$

Note that the left-hand side of (7.3) is equal to

$$\sum_{n=0}^{\infty} \zeta(2n+2)x^{2n} \quad = \quad \frac{1 - \pi x \cot(\pi x)}{2x^2}.$$

Thus, (7.3) generates Apéry-like formulae for $\zeta(2n)$ for every positive in-
teger n. The first few specific instances are

$$\zeta(2) \quad = \quad 3 \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k} k^2},$$

$$\zeta(4) \quad = \quad 3 \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k} k^4} - 9 \sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k-1} j^{-2}}{\binom{2k}{k} k^2},$$

$$\zeta(6) \quad = \quad 3 \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k} k^6} - 9 \sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k-1} j^{-2}}{\binom{2k}{k} k^4} - \frac{45}{2} \sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k-1} j^{-4}}{\binom{2k}{k} k^2}$$

$$+ \frac{27}{2} \sum_{k=1}^{\infty} \sum_{j=1}^{k-1} \frac{\sum_{i=1}^{k-1} i^{-2}}{j^2 \binom{2k}{k} k^2}.$$

We also showed, equivalently, for each positive integer k

$$_3F_2 \left(\begin{array}{c} 3k, -k, k+1 \\ 2k+1, k+\frac{1}{2} \end{array} \middle| \frac{1}{4} \right) \quad = \quad \frac{\binom{2k}{k}}{\binom{3k}{k}}. \qquad (7.4)$$

The proof we gave of (7.4) was via the Wilf-Zeilberger algorithm, and
we requested (other) proofs in the *Monthly* problem section. An attrac-
tive one by Larry Glasser was published recently [146]. It relies on the
elegant representation below in which $P_k^{(k)}$ denotes the *ultra-spherical* or
Gegenbauer polynomial [1]:

$$_3F_2 \left(\begin{array}{c} 3k, -k, k+1 \\ 2k+1, k+\frac{1}{2} \end{array} \middle| x^2 \right) \quad =$$

$$\frac{\Gamma(2k)\Gamma(2k+1)}{\Gamma(k)\Gamma(3k)} \int_0^1 t^k (1-t)^{k-1} P_k^{(k)}(1 - 2x^2 t) \, dt \qquad (7.5)$$

(see Exercise 44). Another solution mathematically performed the Wilf-Zeilberger algorithm.

Here we describe a second "classic" solution of (7.4) by Richard Grivaux that relies on less knowledge of special functions. He starts with a fundamental cubic transformation—due to an earlier one by Bailey [6, p. 185], which is

$$
{}_3F_2 \left(\begin{array}{c} a, 2b - a - 1, a - 2b + 2 \\ b, a - b + \frac{3}{2} \end{array} \middle| \frac{x}{4} \right) \tag{7.6}
$$

$$
= (1 - x)^{-a} {}_3F_2 \left(\begin{array}{c} \frac{a}{3}, \frac{a+1}{3}, \frac{a+2}{3} \\ b, a - b + \frac{3}{2} \end{array} \middle| \frac{-27x}{4(1 - x)^3} \right),
$$

where one sets $a = 3n, b = 2n + 1$. Calling the right-hand hypergeometric $\Delta_n(x)$, we must evaluate $\mathcal{L}_n := \lim_{x \to 1}(1 - x)^{-3n} \Delta_n(x)$. We do this by using the standard representation of ${}_3F_2$ as an integral involving ${}_2F_1$, given, for example, in well-known references ([6, Formula 2.2.2] or [1]). This leads to

$$
\Delta_n(x) = \frac{\Gamma(n + \frac{1}{2})}{\Gamma(n + \frac{2}{3})\Gamma(-\frac{1}{6})} \tag{7.7}
$$

$$
\times \int_0^1 t^{n-1/3}(1 - t)^{7/6} {}_2F_1 \left(\begin{array}{c} n, n + \frac{1}{3} \\ 2n + 1 \end{array} \middle| \frac{-27xt}{4(1 - x)^3} \right) dt.
$$

Moreover, for each n we have

$$
{}_2F_1 \left(\begin{array}{c} n, n + \frac{1}{3} \\ 2n + 1 \end{array} \middle| \frac{-27xt}{4(1 - x)^3} \right)
$$

$$
\sim_{x \to 1} \left(\frac{-27xt}{4(1 - x)^3} \right)^{-n} \frac{\Gamma(2n + 1)\Gamma(\frac{1}{3})}{\Gamma(n + 1)\Gamma(n + \frac{1}{3})} \tag{7.8}
$$

(see, for example, [6, p. 79]).

Putting (7.8) and (7.7) together leads to expressing $\mathcal{L}_n$ as a ratio of Γ-functions multiplied by $(4/27)^n \int_0^1 t^{-1/3}(1 - t)^{-7/6} dt = (4/27)^n \beta(2/3, 1/6)$ (see Section 5.4). The final resolution to $\mathcal{L}_n = \binom{2n}{n}/\binom{3n}{n}$, as in (7.4), is left as Exercise 45.

A further caveat

The following phenomenon is worth mentioning here. Computer packages may be able to sum one expression, but then not another transparently equivalent one. For example, with various specifications of a_m, the series

$$
\sum_{m=0}^n a_m \binom{n}{m}^N \quad \text{and} \quad \sum_{m=0}^\infty a_m \binom{n}{m}^N,
$$

for various powers N may well not return the same answer. In part because
the implicit boundary condition on the right-hand expression may be han-
dled quite differently than that on the left, the two may return different
equivalent expressions—easily seen or not—or one may fail when the other
works. The first two cases are illustrated by the *Maple* session below.

```
Square:=Sum(binomial(n,m)^2,m=0..n) = Sum(binomial(n,m)^2,
  m=0..infinity); value(Square);
```

$$Square := \sum_{m=0}^{n} \text{binomial}(n,\,m)^2 = \sum_{m=0}^{\infty} \text{binomial}(n,\,m)^2$$

returns

$$\frac{4^n\,\Gamma\left(n+\frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(n+1)} = \frac{\Gamma(2\,n+1)}{\Gamma(n+1)^2},$$

whereas

```
Se:=Sum(binomial(n,2*m),m=0..trunc(n/2))=Sum(binomial(n,2*m),
  m=0..infinity): simplify(value(Se));
```

returns *Maple*'s syntax for

$$2^{n-1} - \binom{n}{2+2\lfloor\frac{n}{2}\rfloor} \times$$

$$_3\mathrm{F}_2\left(\begin{array}{c} 1,1-\frac{n}{2}+\lfloor\frac{n}{2}\rfloor,\frac{3}{2}-\frac{n}{2}+\lfloor\frac{n}{2}\rfloor \\ 2+\lfloor\frac{n}{2}\rfloor,\frac{3}{2}+\lfloor\frac{n}{2}\rfloor) \end{array}\middle|1\right) = 2^{n-1},$$

and fails to notice the binomial coefficient is zero. They may indeed some-
times return different answers; see Exercise 10.

Another hypergeometric evaluation

In the spring of 2007, Neil Calkin observed that the $_3F_2$ of (7.5) in the
previous subsection appeared to have structure at 1. For $k = 1, 2, \ldots$ the
values start

$$-\frac{1}{3}, \frac{1}{25}, -\frac{1}{147}, \frac{1}{1089}, -\frac{3}{20449}, \frac{1}{48841}, -\frac{1}{312987}, \frac{25}{55190041},$$
$$-\frac{1}{14322675}, \frac{1}{100100025}.$$

This is exactly the sequence studied in Section 7.1.1. It is quite remarkable
that we have discovered:

$$_3\mathrm{F}_2\left(\begin{array}{c} 6k, -2k, 2k+1 \\ 4k+1, 2k+\frac{1}{2} \end{array}\middle|1\right) = \left(\frac{(4k)!(3k)!}{(6k)!(k)!}\right)^2 \tag{7.9}$$

and

$$
{}_3\mathrm{F}_2\left(\begin{array}{c} 6k+3, -2k-1, 2k+2 \\ 4k+3, 2k+\frac{3}{2} \end{array}\middle|1\right) = -\frac{1}{3}\left(\frac{(4k+1)!(3k)!}{(6k+1)!(k)!}\right)^2 \tag{7.10}
$$

both essentially squares of binomial ratios. Each can be proven with a little nursing by Zeilberger's algorithm. Here is the *Maple* code for the even case:

```
with(SumTools[Hypergeometric]): rf:=proc(a,b):(a+b-1)!/(a-1)!:end:
F:=rf(-m,k)*rf(3*m,k)*rf(m+1,k)/rf(2*m+1,k)/rf(m+1/2,k)/k!:
F:=subs(m=2*m,F): a:=1/(6*m)!/m!*(4*m)!*(3*m)!;F:=F/a^2:
ts:=time();jb:=Zeilberger(F,m,k,M): ope:=jb[1]: print('The operator
annihilating the left normalized by dividing by the right is'):
print(ope): print('The proof (certificate) can be found by doing
jb[2]; (but I spare you)'): print('The constant sequence is
annihilated by the above-mentioned operator since'):
print('plugging-in M=1, gives 0, indeed doing it '):
print(subs(M=1,jb[1])): print('and the statement follows by
induction by checking it for m=0, m=1 '): print('QED'): print('This
took', time()-ts, 'seconds  of CPU time '):
```

The odd case may be similarly established.

Mizan Rahman has provided a very clean conventional proof, the discovery of which requires significant familiarity with generalized hypergeometric series. We sketch the even case of (7.9). We start by using two transformation formulas for ${}_3F_2$:

$$
{}_3\mathrm{F}_2\left(\begin{array}{c} 3n, -n, n+1 \\ 2n+1, n+\frac{1}{2} \end{array}\middle|1\right) = (-1)^n {}_3\mathrm{F}_2\left(\begin{array}{c} 3n, -n, n \\ 2n+1, n+\frac{1}{2} \end{array}\middle|1\right)
$$
$$\tag{7.11}$$

(see [143, (3.1.1)]), and

$$
{}_3\mathrm{F}_2\left(\begin{array}{c} 3n, -n, n \\ 2n+1, n+\frac{1}{2} \end{array}\middle|1\right) = \frac{(n+1)_n}{(2n+1)_n} {}_3\mathrm{F}_2\left(\begin{array}{c} -n, \frac{1}{2}-2n, n \\ -2n, n+\frac{1}{2} \end{array}\middle|1\right)
$$
$$\tag{7.12}$$

(see [6, p. 142]). Here $(a)_n := a(a+1)\cdots(a+n-1) = \Gamma(a+n)/\Gamma(a)$ denotes the *rising factorial*.

We also invoke a special case of *Whipple's formula*, (see [261, 2.4.2.3]), which yields a seemingly more complicated ${}_4\mathrm{F}_3$

$$
{}_3\mathrm{F}_2\left(\begin{array}{c} -n, \frac{1}{2}-2n, n \\ -2n+1, n+\frac{1}{2} \end{array}\middle|1\right) = \frac{(-3n)_n}{(-2n)_n} {}_4\mathrm{F}_3\left(\begin{array}{c} n+1, -\frac{n}{2}, n, \frac{3n}{2} \\ n+1, n+\frac{1}{2}, n+\frac{1}{2} \end{array}\middle|1\right)
$$
$$\tag{7.13}$$

The $(n+1)$ terms cancel, however, and leave a so-called *balanced* $_3F_2$, to which the *Pfaff-Saalschútz identity* (see [6, Theorem 2.2.6]) applies, since $n = 2k$ is even:

$$_3F_2 \left(\begin{array}{c} -k, a, b \\ c, 1 + a + b - c - k \end{array} \middle| 1 \right) = \frac{(c-a)_k (c-b)_k}{(c)_k (c-a-b)_k}. \tag{7.14}$$

We leave it as Exercise 46 to confirm that this results in

$$_3F_2 \left(\begin{array}{c} 3n, -n, n+1 \\ 2n+1, n+\frac{1}{2} \end{array} \middle| 1 \right) = \left(\frac{\left(\frac{1}{2}\right)_{n/2}}{\left(\frac{1}{2}+n\right)_{n/2}} \right)^2, \tag{7.15}$$

for even n and that this is equivalent to (7.9).

7.1.5 Changing Representations

Suppose we are presented with a sequence of power series whose first three elements are:

$$
\begin{aligned}
S_1 \quad := \quad & 1 - x^3 + 2\,x^4 - 2\,x^7 + 4\,x^8 - 4\,x^{11} + 8\,x^{12} - 8\,x^{15} + 16\,x^{16} - 16\,x^{19} \\
& + 32\,x^{20} - 32\,x^{23} + 64\,x^{24} - 64\,x^{27} + 128\,x^{28} - 128\,x^{31} + 256\,x^{32} \\
& - 256\,x^{35} + 512\,x^{36} - 512\,x^{39} + 1024\,x^{40} - 1024\,x^{43} + 2048\,x^{44} \\
& - 2048\,x^{47} + 4096\,x^{48} - 4096\,x^{51} + 18192\,x^{52} - 8192\,x^{55} \\
& + 16384\,x^{56} - 16384\,x^{59} + 32768\,x^{60} + O\left(x^{63}\right) \tag{7.16}
\end{aligned}
$$

$$
\begin{aligned}
S_2 \quad := \quad & 1 - x^3 + 2\,x^4 - x^6 + 4\,x^8 + x^9 - 4\,x^{10} + 8\,x^{12} - 4\,x^{14} + 18\,x^{16} \\
& - 4\,x^{17} - 8\,x^{18} + 32\,x^{20} - 16\,x^{22} + 4\,x^{23} + 56\,x^{24} - 32\,x^{26} \\
& + 128\,x^{28} - 56\,x^{30} - 16\,x^{31} + 256\,x^{32} - 128\,x^{34} + 512\,x^{36} + 16\,x^{37} \\
& - 288\,x^{38} + 1024\,x^{40} - 512\,x^{42} + 2080\,x^{44} - 64\,x^{45} - 1024\,x^{46} \\
& + 4096\,x^{48} - 2048\,x^{50} + 64\,x^{51} + 8064\,x^{52} + 4096\,x^{54} \\
& + 16384\,x^{56} - 8064\,x^{58} - 256\,x^{59} + 32768\,x^{60} + O\left(x^{61}\right) \tag{7.17}
\end{aligned}
$$

$$
\begin{aligned}
S_3 \quad := \quad & 1 - x^3 + 2\,x^4 - x^6 + 4\,x^8 - 2\,x^{10} + 9\,x^{12} - 4\,x^{13} + x^{15} + 16\,x^{16} \\
& - 8\,x^{17} - x^{18} + 4\,x^{19} + 28\,x^{20} - 8\,x^{21} + 2\,x^{22} + 56\,x^{24} - 16\,x^{25} \\
& + 4\,x^{26} - 8\,x^{27} + 126\,x^{28} - 24\,x^{29} - 16\,x^{31} + 256\,x^{32} - 56\,x^{33} \\
& - 16\,x^{34} + 520\,x^{36} - 128\,x^{37} - 36\,x^{38} + 8\,x^{39} + 1040\,x^{40} - 288\,x^{41} \\
& + 16\,x^{43} + 2048\,x^{44} - 576\,x^{45} + 32\,x^{47} + 4024\,x^{48} - 1008\,x^{49} \\
& + 32\,x^{50} + 8064\,x^{52} - 2048\,x^{53} + 64\,x^{54} - 128\,x^{55} + 16384\,x^{56} \\
& - 4032\,x^{57} - 16\,x^{58} - 224\,x^{59} + 32768\,x^{60} + O\left(x^{61}\right). \tag{7.18}
\end{aligned}
$$

We may or may not have a closed form for the series coefficients, but in any event no pattern is clear or even appetizing. If, however, we define p in *Maple* as follows, and run the subsequent three lines of code:

```
>  p:=numapprox[pade];
>  factor(numapprox[pade](S[1],x,[10,10]));
```

$$\frac{(x-1)\,(x^2+x+1)}{2\,x^4-1}$$

```
>  factor(numapprox[pade](S[2],x,[20,20]));
```

$$\frac{(x^2-x+1)\,(x+1)\,(x-1)^2\,(x^2+x+1)^2}{(2\,x^4-1)\,(2\,x^7-1)}$$

```
>  factor(numapprox[pade](S[3],x,[30,30]));;
```

$$\frac{(x+1)\,(x^2-x+1)\,(x^6+x^3+1)\,(x-1)^3\,(x^2+x+1)^3}{(2\,x^{10}-1)\,(2\,x^4-1)\,(2\,x^7-1)}$$

.

This will certainly spot the pattern

$$S_N = \frac{\prod_{k=1}^{N}\left(1-x^{3\,k}\right)}{\prod_{k=1}^{N}\left(1-2\,x^{3\,k+1}\right)}.$$

In fact the original sequence was generated from the *Maple* code

```
R:=N->product(1-x^(3*k),k=1..N)/product(1-2*x^(3*k+1),
k=1..N): for j to 5 do S[j]:=series(R(j),x,61) od:
```

Other such modalities

Other useful representation changes include continued fractions, base change, partial fractions, matrix decompositions, and many more. In each case, the computer has revolutionized our ability to exploit them. And with each problem, the key first question is: what other representation might expose more structure?

   We illustrate the first two of these here and leave the others as Exercises. In the following examples, we start each time with a decimal expansion and ask what it is. Of course, we might also use the inverse calculator or identify utility, but let us initially eschew its use.

  - *Continued Fractions.* The unmemorable

    $$\alpha := 1.43312742672231175831718345577599182043151527679060\ldots$$

when converted to a simple continued fraction reveals

$$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$$

Now one certainly can ask a better question: what numbers have such arithmetic continued fractions? The answer will be found in all good books on the subject. Alternatively, searching for *arithmetic, progression, continued fraction,* in Google returned

`http://mathworld.wolfram.com/ContinuedFractionConstant.html`

which tells us, among many other salient things, that

$$[A + D, A + 2D, A + 3D, \ldots] \quad = \quad \frac{I_{A/D}\left(\frac{2}{D}\right)}{I_{1+A/D}\left(\frac{2}{D}\right)}$$

for real A and nonzero D. Here, I_s is the *modified Bessel function of the first kind.* In particular, we have discovered $I_0(2)/I_1(2)$.

This is also achieved if we enter the sequence $1, 4, 3, 3, 1, 2, 7, 4, 2, 6, 7, 2$ into Sloane's Encyclopedia. We recover, in sequence A060997, the continued fraction, its Bessel representation (and series definition), along with the following *Mathematica* code.

```
RealDigits[ FromContinuedFraction[ Range[ 44]], 10, 110] [[1]]
(*Or*) RealDigits[ BesselI[0, 2] / BesselI[1, 2], 10, 110] [[1]]
(*Or*) RealDigits[ Sum[1/(n!n!), {n, 0, Infinity}]
/ Sum[n/(n!n!), {n, 0, Infinity}], 10, 110] [[1]]
```

Similarly

$\quad \beta := 12.76714533480370466171095200978089234738236378030112588$

yields

$$[12, 1, 3, 3, 2, 1, 1, 7, 1, 11, 1, 7, 1, 1, 2, 3, 3, 1, 24, 1, 3, 3, 2, 1, 1, 7, 1, 11,$$
$$1, 7, 1, 1, 2, 3, 3, 1, 24, 1, 3, 3, 2, 1, 1, 7, 1, 11, 1, 7, 1, 1, 2, 3, 3, 1, 24, \cdots]$$

which appears to be periodic albeit with a long period. Another famous result of Lagrange says eventually periodic continued fractions correspond to real quadratic irrationalities. So we square and obtain

$\quad\quad 162.9999999999999999999999999999999999999999999999.$

This last step would be slightly more challenging if we had started with $\beta - 12$. Now *Maple* via `identify` $(\beta - 12)$; returns $\sqrt{163} - 12$, whereas `with(PolynomialTools):MinimalPolynomial` $(\beta - 12, 2)$; returns the corresponding quadratic equation. We leave identification of

$\quad \delta := 1.4102787972078658917940430244710631444834239245953$

Figure 7.2. Matrix plots of the continued fractions for e (left) and π (right).

Figure 7.3. Matrix plots of the decimal expansions for e (left), π (center) and $22/7$ (right).

as Exercise 21.

Figure 7.1.5 shows 4350 terms of the simple continued fractions for e and π (truncated at 12) as matrix plots. Correspondingly, Figure 7.1.5 shows 10,000 terms of the decimal expansions for e, π and $22/7$. The goal is not to show fine structure, but rather how qualitative differences jump out at one visually. For an up-to-date philosophical and cognitive accounting of the role and nature of visual thinking in mathematics, we point the reader to Giaquinto [145] for whom "discovering a truth is coming to believe it in an independent, reliable, and rational way." (This definition encompasses rediscovery [145, p. 50].)

- *Base Change.* Consider the numbing binary integer

$$\mu \quad := \quad 1111100101010001101010011111110100111100000101010110$$
$$001010111111011111111110000100010101011100011100000$$

In decimal form, it becomes memorable:

$$1234567891011121314151617181920.$$

Now consider the related *Champernowne number*

$$\lambda := 0.12345678910111213141516171819202021\ldots$$

which is provably normal in base ten. Its continued fraction begins with the sequence $[0, 8, 9, 1, 149083, 1, 1, 1, 4$ and continues

$$1, 1, 1, 3, 4, 1, 1, 1, 15, 4534684669364804044938725073405 20808, 2].$$

This is explored further in Exercises 34 and 48.

In his recent book *Mathematics and Common Sense* [124], Philip Davis deals explicitly and engagingly with many of the same themes as we tackle here. In particular, his essays on the nature of mathematical intuition, proof, visualization and much more make an excellent counterpoint to the current, more technical discussion. Equally, Terence Tao's brief book *Solving Mathematical Problems* [274] is a fine addition to the corpus.

7.2   Recursions for Ising Integrals

The main aim of this section, which follows that given by Borwein and Salvy [79] closely, is twofold. First, we shall prove a conjecture concerning the existence of a recurrence in $k \geq 0$ satisfied by the integrals

$$
\begin{aligned}
C_n &:= \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^{k+1}} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n} \\
&= \frac{1}{n!} \int_0^\infty \cdots \int_0^\infty \frac{dx_1 dx_2 \cdots dx_n}{(\cosh x_1 + \cdots + \cosh x_n)^{k+1}},
\end{aligned}
$$

for $n = 1, 2, \ldots$ (see [28, 22]). These integrals naturally arose during the analysis of parts of the Ising theory of solid-state physics [28]. In a previous discussion [22], only the first four cases of Theorem 7.0 were proven, and the proofs relied on the ability to express the corresponding integrals in (7.21) as *Meijer G-functions*, something that fails for $n > 4$.

A second aim is to advertise the power of current symbolic computational tools and related algorithmic developments to settle such questions. For this reason, we offer a quite detailed exposition of the methods entailed.

Our main result (Theorem 7.0) is better phrased in terms of

$$c_{n,k} := \frac{n! \Gamma(k+1)}{2^n} C_{n,k}. \tag{7.19}$$

Theorem 7.64. *(Linear Recursion) For any fixed $n \in \mathbb{N}$, the sequence $c_{n,k}$ possesses a linear recurrence with polynomial coefficients of the form*

$$(k+1)^{n+1} c_{n,k} + \sum_{\substack{2 \leq j < n \\ j \text{ even}}} P_{n,j}(k) c_{n,k+j} = 0, \tag{7.20}$$

with $\deg P_{n,j} \leq n+1-j$.

Substituting (7.19) and simplifying by $n!\Gamma(k+1)/2^n$ yields

$$(k+1)^{n+1}C_{n,k} + \sum_{\substack{2 \leq j < n \\ j \text{ even}}} P_{n,j}(k)(k+j)(k+j-1)\cdots(k+1)C_{n,k+j} \quad = \quad 0,$$

which is Conjecture 1 of an earlier publication of ours [22], with extra information added on the origin of the linear factors for the recurrence in $C_{n,k}$.

The starting point of our proof is the integral representation [22, Equation (8)]

$$c_{n,k} \quad = \quad \int_0^{+\infty} t^k K_0(t)^n \, dt, \tag{7.21}$$

where K_0 is the *modified Bessel function* on which much information is offered elsewhere [1, Chapter 9]. The key properties of K_0 that we use here are as follows. First,

$$K_0(t) \quad = \quad \int_0^{\infty} e^{-t\cosh(x)} \, dx,$$

which explains how the integrals in (7.21) arise. Moreover, we have

- a linear differential equation: $(\theta^2 - t^2)K_0(t) = 0$ with $\theta := t \, d/dt$;

- the behavior at the origin: $K_0(t) \sim -\ln t$, $t \to 0$;

- and the behavior at infinity: $K_0(t) \sim \sqrt{\pi/2t}e^{-t}$, $t \to +\infty$.

These last two properties show that the integral (7.21) converges for any complex k subject to $\mathrm{Re}(k) > -1$ where it defines an analytic function of k. The recurrence of Theorem 7.0 then gives the integral a meromorphic continuation to the whole complex plane with poles at the negative integers.

7.2.1 Existence of a Recurrence

The theory of D-finite series leads to a direct proof of existence of a recurrence such as (7.20) in a very general setting, together with an algorithm.

Recall that a power series is called *D-finite* when it satisfies a linear differential equation with polynomial coefficients. Stanley offers a good introduction to the basic properties of these series [264]. What makes these series appealing from the algorithmic point of view is that they exist

in finite-dimensional vector spaces, and thus many of their properties can be explicitly computed by linear algebra in finite dimensions. In this setting, Proposition$N$ 7.0 is easily obtained. It is a generalization of our main Theorem 7.0, except for the absence of degree bounds.

Proposition 7.65. *Assume that $f(t)$ obeys a homogeneous linear differential equation*

$$a_r(t)f^{(r)}(t) + \cdots + a_0(t)f(t) = 0,$$

with polynomial coefficients $a_i(t)$ in $\mathbb{C}[t]$. For a fixed $n \in \mathbb{N} \setminus \{0\}$, let Γ be a path in $\mathbb{C}$ such that for any $k \in \mathbb{N}$, the integrals

$$I_k := \int_\Gamma t^k f(t)^n \, dt$$

converge and the limits of the integrand at both endpoints coincide. Then the sequence $\{I_k\}$ obeys a linear recurrence with coefficients that are polynomial in n and k and that can be computed given the coefficients a_i.

We give the proof in two steps. The first one is classic [264, Theorem 6.4.9].

Lemma 7.66. *D-finite series form an algebra over the rational functions.*

This means that any polynomial in D-finite series with rational function coefficients defines a series that is itself D-finite. In particular, K_0^n satisfies a linear differential equation.

Proof. The proof is effective. The difficult part is the product. The derivatives of two D-finite functions f and g exist in finite-dimensional vector spaces generated by $f, \ldots, f^{(r-1)}$ and $g, \ldots, g^{(s-1)}$. Therefore, by repeated differentiation, the derivatives of a product $h := fg$ can be rewritten as linear combinations of the terms $f^{(i)}g^{(j)}$, $0 \le i < r$, $0 \le j < s$, which generate a vector space of dimension at most rs. It follows that the $rs + 1$ successive $h^{(k)}$, $k = 0, \ldots, rs$, are linearly dependent. A linear dependency between them can be found as the kernel of the linear map $(\lambda_0, \ldots, \lambda_{rs}) \mapsto \lambda_0 h + \cdots + \lambda_{rs}h^{(rs)}$. Any such linear dependency is a linear differential operator annihilating fg. $\square$

The corresponding algorithm is implemented, among other places, in the *Maple* package gfun [252].

Example 7.67. Here is how the function `gfun[poltodiffeq]` is invoked to compute a differential equation for K_0^4:

```
> eqK0:=t*diff(t*diff(y(t),t),t)-t^2*y(t);
```

$$eqK0 \quad := \quad t(t\frac{d^2}{dt^2}y(t) + \frac{d}{dt}y(t)) - t^2 y(t)$$

```
> gfun[poltodiffeq](y(t)^4,[eqK0],[y(t)],y(t))=0;
```

$$t^4\frac{d^5}{dt^5}y(t) + 10t^3\frac{d^4}{dt^4}y(t) - (20t^4 - 25t^2)\frac{d^3}{dt^3}y(t)$$

$$-(120t^3 - 15t)\frac{d^2}{dt^2}y(t) + (64t^4 - 152t^2 + 1)\frac{d}{dt}y(t) + (128t^3 - 32t)y(t) = 0$$

Example 7.68. The corresponding steps of the calculation for the smaller example K_0^2 are presented here:

$$
\begin{aligned}
h &= K_0^2, \\
h' &= 2K_0 K_0', \\
h'' &= 2K_0'^2 - 2t^{-1}K_0 K_0' + 2K_0^2, \\
h^{(3)} &= -6t^{-1}K_0'^2 + 4(2 + t^{-2})K_0 K_0' - 2t^{-1}K_0^2,
\end{aligned}
$$

where, whenever possible, we have replaced K_0'' by $K_0 - t^{-1}K_0'$. Then we find the vector $(-4t, 1 - 4t^2, 3t, t^2)$ in the kernel of

$$
\begin{matrix}
1 & 0 & 2 & -2t^{-1} \\
0 & 2 & -2t^{-1} & 4(2 + t^{-2}) \\
0 & 0 & 2 & -6t^{-1}
\end{matrix} \quad . \tag{7.22}
$$

This vector then produces a differential equation satisfied by K_0^2:

$$t^2 y^{(3)} + 3ty'' + (1 - 4t^2)y' - 4ty \quad = \quad 0.$$

Proof (continued). The second step of the proof of Proposition 7.0 starts by expanding the differential equation for $h := f^n$ as

$$\sum_{i,j} d_{i,j} t^i h^{(j)} \quad = \quad 0,$$

for scalars $d_{i,j}$. This is then multiplied by t^k and integrated along Γ. Use of the convergence hypotheses then allows us to deduce that

$$\sum_{i,j} d_{i,j} \int_\Gamma t^{k+i} h^{(j)} \, dt \quad = \quad 0. \tag{7.23}$$

Integration by parts now yields

$$
\int_\Gamma t^{k+i} h^{(j)}\, dt \;\; = \;\; \underbrace{t^{k+i} h^{(j-1)}\Big|_\Gamma}_{0} - (k+i)\int_\Gamma t^{k+i-1} h^{(j-1)}\, dt,
$$

$$
= \;\; (-k-i)(-k-i+1)\cdots(-k-i+j-1) I_{k+i-j},
$$

the last equality following by induction. Adding the contributions of all the terms in (7.23) finally yields the desired recurrence over I_k. $\qquad\square$

Example 7.69. For $h := K_0^2$, the computation gives

$$
\int_0^{+\infty} t^{k+2} h^{(3)} + 3 t^{k+1} h'' + (t^k - 4 t^{k+2}) h' - 4 t^{k+1} h\, dt \;\; = \;\; 0,
$$

from which we obtain

$$
(-k-2)(-k-1)(-k) c_{2,k-1} + 3(-k-1)(-k) c_{2,k-1}
$$
$$
+(-k) c_{2,k-1} - 4(-k-2) c_{2,k+1} - 4 c_{2,k+1} \;\; = \;\; 0.
$$

Once simplified, this reduces to

$$
4(k+1) c_{2,k+1} \;\; = \;\; k^3 c_{2,k-1}. \tag{7.24}
$$

Mellin transform

As the proof indicates, Proposition 7.0 is not restricted to integer values of k. In particular, the method gives a difference equation for the *Mellin transform*

$$
h^\star(s) \;\; := \;\; \int_0^{+\infty} t^{s-1} h(t)\, dt,
$$

provided the appropriate convergence properties are satisfied. This difference equation then gives a meromorphic continuation in the whole complex plane. The most basic example is $\Gamma(s)$: starting from the elementary differential equation $y' + y = 0$ for $h(t) = \exp(-t)$ leads to the classic functional equation $\Gamma(s+1) = s\Gamma(s)$.

Coefficients

The path Γ can also be a closed contour. For instance, if h is analytic at the origin, then the kth coefficient of its Taylor series at the origin is given by the Cauchy integral

$$\frac{1}{2\pi i} \oint \frac{h(t)}{t^{k+1}}\, dt,$$

where the contour encloses the origin and no other singularity of h. The algebraic manipulations are the same as in the previous case, followed by replacing k by $-k-1$ and the sequence c_k by the sequence u_{-k-1}.

For instance, if we apply this transform to the functional equation for Γ, we first get $c_{-s} = -sc_{-s-1}$ and then $u_{s-1} = -su_s$, which is the expected recurrence for the sequence of coefficients $u_s = (-1)^s/s!$ of $\exp(-t)$.

Similarly, starting from (7.24), we obtain the mirror recurrence

$$4k\tilde{c}_{k-1} \quad = \quad (k+1)^3\tilde{c}_{k+1}.$$

Observe that this is obeyed by the coefficients of $\ln^2(t)$ in the series expansion

$$
\begin{aligned}
K_0^2(t) \quad = \quad & \ln^2(t)\left(1 + \frac{1}{2}t^2 + \frac{3}{32}t^4 + \frac{5}{576}t^6 + \dots\right) \\
& + \ln(t)\left(2\gamma - 2\ln 2 + \left(\gamma - \ln 2 - \frac{1}{2}\right)t^2 + \dots\right) \\
& + \left((\ln 2 - \gamma)^2 + \dots\right), \quad t \to 0^+.
\end{aligned}
$$

The Frobenius computation of expansions of solutions of linear differential equations at regular singular points (see, e.g., [174]) explains why this is so.

In sum, all these algorithms succeed in making effective and efficient the familiar method of differentiation under the integral sign and integration by parts. Further discussion can be found in Exercises 11 and 12.

7.2.2 Proof of the Main Result on Recursions

If A is a linear differential operator, the operator of minimal order that annihilates the nth power of every solution of A is called its nth *symmetric power*. Because of its role in algorithms for differential Galois theory [281] there has been interest in efficient algorithms computing symmetric powers. In the case of *second-order* operators, such an algorithm has been found [98]. We state it in terms of the derivation $\theta := t\,d/dt$ to get better control

over the coefficients of the resulting recurrence—but the statement and proof hold for any derivation.

Lemma 7.70. *(Linear Differential Equation, [98].) Let $A = \theta^2 + a(t)\theta + b(t)$ be a linear differential operator with rational function coefficients $a(t)$ and $b(t)$. Let $L_0 = 1$, $L_1 = \theta$, and define the operator L_{k+1} for $k = 1, 2, \ldots, n$ by*

$$L_{k+1} \quad := \quad (\theta + ka)L_k + bk(n - k + 1)L_{k-1}. \tag{7.25}$$

Then, for $k = 0, \ldots, n + 1$, and for an arbitrary solution y of $Ay = 0$,

$$L_k y^n = n(n - 1) \cdots (n - k + 1) y^{n-k} (\theta y)^k,$$

and in particular $L_{n+1} y^n = 0$.

(This recursion can be viewed as an efficient computation of the kernel which was described in the previous section, taking advantage of the special structure of the current matrix.)

Proof. The proof is a direct verification by induction. For $k = 0$ and $k = 1$, the identity reduces, respectively, to $y^n = y^n$ and $\theta y^n = ny^{n-1}\theta(y)$, which are obviously true for any function y. Assuming the identity to hold up to $k \geq 1$, the heart of the induction is the rule for differentiation of a product $\theta(uv) = \theta(u)v + u\theta(v)$:

$$
\begin{aligned}
\theta(y^{n-k}(\theta y)^k) &= \theta(y^{n-k})(\theta y)^k + y^{n-k}\theta((\theta y)^k) \\
&= (n - k)y^{n-k-1}(\theta y)^{k+1} + ky^{n-k}(\theta y)^{k-1}(\theta^2 y) \\
&= (n - k)y^{n-k-1}(\theta y)^{k+1} + ky^{n-k}(\theta y)^{k-1}(a\theta y + by).
\end{aligned}
$$

Reorganizing terms concludes the induction.   □

Example 7.71. In the case of K_0, we have $a = 0$ and $b = -t^2$. For $n = 4$, starting with $L_0 = 1$ and $L_1 = \theta$, the recurrence of Lemma 7.0 gives

$$
\begin{aligned}
L_2 &= \theta^2 - 4t^2, \\
L_3 &= \theta^3 - 10t^2\theta - 8t^2, \\
L_4 &= \theta^4 - 16t^2\theta^2 - 28t^2\theta + 8t^2(3t^2 - 2), \\
L_5 &= \theta^5 - 20t^2\theta^3 - 60t^2\theta^2 + 8t^2(8t^2 - 9)\theta + 32t^2(4t^2 - 1).
\end{aligned}
$$

The operator L_5 annihilates K_0^4. It is a rewriting in terms of θ of the equation of Example 7.0.

Some of the patterns that emerge on this example can be proven in the general case.

Lemma 7.72. *(Closed Form.) With the same notation as in Lemma 7.0, when $A = \theta^2 - t^2$, L_k may be written as*

$$L_k \;=\; \theta^k + \sum_{j=0}^{k-2} a_j^{(k)}(t)\theta^j,$$

where each $a_j^{(k)}$ is a polynomial in t^2, divisible by t^2 and $\deg a_j^{(k)} \le k - j$.

Proof. Again, the proof is by induction. For $k = 0$ and $k = 1$, we recover the definition of L_0 and L_1. For larger k, the recurrence (7.25) simplifies to

$$L_{k+1} \;:=\; \theta L_k - k(n - k + 1)t^2 L_{k-1}.$$

If the property holds up to $k \ge 1$, then this shows that the degree of L_{k+1} in θ is $k + 1$, with leading coefficient 1, and also that the coefficient of θ^k in L_{k+1} is 0. Extracting the coefficient of θ^j then gives

$$a_j^{(k+1)} \;=\; \begin{cases} a_{j-1}^{(k)} + \theta(a_j^{(k)}) - k(n - k + 1)t^2 a_j^{(k-1)}, & 0 \le j \le k - 2, \\ -k(n - k + 1)t^2, & j = k - 1. \end{cases}$$

These last two identities give the desired degree bound and divisibility property for the coefficients $a_j^{(k+1)}$, $0 \le j \le k - 1$.   □

We may now complete the proof of the main result.

Proof of Theorem 7.0. Lemma 7.0 shows that the coefficients of L_{n+1} can be rewritten as

$$L_{n+1} \;=\; \theta^{n+1} + \sum_{\substack{2 \le j < n \\ j \text{ even}}} t^j Q_j(\theta), \tag{7.26}$$

where the polynomials Q_j satisfy $\deg Q_j \le n + 1 - j$.

Thanks to the properties of K_0 recalled earlier in this section, an integration by parts yields

$$\int_0^{+\infty} t^{k+j}\theta^m (K_0^n(t))\, dt \;=\; (-1 - k - j)^m c_{n,k+j}, \tag{7.27}$$

for each m. Now we multiply $L_{n+1}K_0^n$ from (7.26) by t^k and integrate from 0 to infinity:

$$\int_0^\infty \left\{ t^k \theta^{n+1} K_0^n(t) + \sum_{\substack{2 \le j < n \\ j \text{ even}}} t^{k+j} Q_j(\theta) K_0^n(t) \right\} dt \;=\; 0.$$

Integrating term by term and using (7.27) finally gives the recurrence

$$(-k-1)^{n+1} c_{n,k} + \sum_{\substack{2 \le j < n \\ j \text{ even}}} Q_j(-1-k-j) c_{n,k+j} \;=\; 0,$$

which is the desired one, up to renaming and sign changes.   □

7.2.3   Algorithm for Recursions

In summary, we have a relatively straightforward algorithm to compute the linear recurrences for the $c_{n,k}$ or $C_{n,k}$ for given n. First, the operators L_k can be computed as *commutative* polynomials $\tilde{L}_k$ as follows:

$$\tilde{L}_{k+1} \;:=\; t\frac{\partial \tilde{L}_k}{\partial t} + \theta \tilde{L}_k - k(n-k+1)t^2 \tilde{L}_{k-1}, \quad 1 \le k \le n, \;(7.28)$$

with initial values $\tilde{L}_0 := 1$ and $\tilde{L}_1 := \theta$. These polynomials $\tilde{L}_k$ coincide with the operators L_k when the powers of θ are written on the *right* of the monomials in t and θ.

By collecting coefficients of t in $\tilde{L}_{n+1}$, we recover (7.26). Substituting $-1-k-j$ for θ in the coefficient of t^j then produces the desired recurrence for $c_{n,k}$, and replacing $c_{n,k+j}$ by $(k+1)\cdots(k+j)C_{n,k+j}$ for all j produces the desired recurrence for $C_{n,k}$.

Example 7.73. We illustrate the process for $n = 4$. The last operator in Example 7.0 may be rewritten as

$$L_5 \;=\; \theta^5 - 4t^2(5\theta^3 + 15\theta^2 + 18\theta + 8) + 64t^4(\theta + 2)$$

and annihilates $K_0^4(t)$. Substituting $-1-k-j$ for θ in the coefficient of t^j for $j = 0, 2, 4$ gives

$$-(k+1)^5 c_{4,k} + 4(k+2)(5k^2 + 20k + 23)c_{4,k+2} - 64(k+3)c_{4,k+4} \;=\; 0.$$

Since $c_{4,k} = \frac{3}{2}\Gamma(k+1)C_{4,k}$, this is equivalent to

$$-\frac{3}{2}(k+1)^4 C_{4,k} + 6(k+2)^2(5k^2 + 20k + 23)C_{4,k+2}$$
$$-96(k+4)(k+3)^2(k+2)C_{4,k+4} \quad = \quad 0,$$

which has been proven by different methods elsewhere [22].

Here is the corresponding *Mathematica* code, courtesy of Manuel Kauers and Veronika Pillwein [183]:

```
ComputeQ[n_, theta_, t_] := Module[{k, L},
  L[0] = 1; L[1] = theta;
  Do[
   L[k + 1] =
    Expand[t*D[L[k], t] + L[k] theta - k (n-k+1) t^2 L[k - 1]]
   , {k, 1, n}];
  L[n + 1]
  ];
recc[c_, n_Integer, k_] := Module[{Q, theta, t, j},
 Q = ComputeQ[n, theta, t];
 Sum[Factor[Coefficient[Q, t, j] /. theta -> -1 - k - j]
   c[n, k + j], {j, 0, n + 1}]]
recC[c_, n_Integer, k_] := Module[{Q, theta, t, j, ell},
 Q = ComputeQ[n, theta, t];
 (-1)^(n + 1) (k + 1)^n c[n, k] +
  Sum[Factor[Coefficient[Q, t, j] /. theta -> -1 - k - j]
    Pochhammer[k + 2, j - 1] c[n, k + j], {j, 1, n + 1}]]
```

On a 2007-era personal computer, all recurrences for n up to 100 can be obtained in a few minutes. Further time could be saved by not factoring the coefficients. Using the *Mathematica* code given above, the recursions for $c_{4,k}$ and $C_{4,k}$ may be determined by the commands `recc[c,4,k]` and `recC[c,4,k]`, respectively, which yield

$$-(k+1)^5 c_{4,k} + 4(k+2)(5k^2 + 20k + 23)c_{4,k+2} - (64k + 192)c_{4,k+4} \quad = \quad 0$$
$$-(k+1)^4 C_{4,k} + 4(k+2)^2(5k^2 + 20k + 23)C_{4,k+2}$$
$$-64(k+4)(k+3)^2(k+2)C_{4,k+4} \quad = \quad 0,$$

respectively. The first six cases for $C_{n,k}$ are

$$0 \;=\; (k+1)C_{1,k} - (k+2)C_{1,k+2} \tag{7.29}$$

$$0 \;=\; (k+1)^2 C_{2,k} - 4(k+2)^2 C_{2,k+2} \tag{7.30}$$

$$0 \;=\; (k+1)^3 C_{3,k} - 2(k+2)\left(5(k+2)^2 + 1\right)C_{3,k+2}$$
$$+9(k+2)(k+3)(k+4)C_{3,k+4} \tag{7.31}$$

$$0 \;=\; (k+1)^4 C_{4,k} - 4(k+2)^2(5(k+2)^2 + 3)C_{4,k+2}$$
$$+64(k+2)(k+3)^2(k+4)C_{4,k+4} \tag{7.32}$$

$$0 \;=\; (k+1)^5 C_{5,k} - (k+2)\left(35k^4 + 280k^3 + 882k^2 + 1288k + 731\right)C_{5,k+2}$$
$$+(k+2)(k+3)(k+4)\left(259k^2 + 1554k + 2435\right)C_{5,k+4}$$
$$-225(k+2)(k+3)(k+4)(k+5)(k+6)C_{5,k+6} \tag{7.33}$$

$$0 \;=\; (k+1)^6 C_{6,k} - 8(k+2)^2\left(7k^4 + 56k^3 + 182k^2 + 280k + 171\right)C_{6,k+2}$$
$$+16(k+2)(k+3)^2(k+4)\left(49k^2 + 294k + 500\right)C_{6,k+4}$$
$$-2304(k+2)(k+3)(k+4)^2(k+5)(k+6)C_{6,k+6}. \tag{7.34}$$

as given by Bailey, Borwein, Borwein, and Crandall [22], but in which only the first four were proven. Many more recursions were determined empirically, by using integer relation methods—this relied on being able to compute the integrals in (7.21) to very high precision—and led to the now-proven conjecture.

Implicit in this algorithm is an explicit recursion for the polynomial coefficients of each recursion. In the case of (7.31) and (7.32), these recursions led to new continued fractions for $L_{-3}(2)$ and $\zeta(3)$, respectively [28, 22]. These rely additionally on the facts that $C_{3,1} = L_{-3}(2), C_{3,3} = 2\,L_{-3}(2)/9 - 4/27$ and $C_{4,1} = 7\,\zeta(3)/12, C_{4,3} = 7\,\zeta(3)/288 - 1/48$, [22].

7.2.4   Another Example

In a paper with Crandall [27] (to which we refer for motivation and references), we considered the following "box integrals":

$$B_n(s) \;=\; \int_0^1 \cdots \int_0^1 (r_1^2 + \cdots + r_n^2)^{s/2}\, dr_1 \cdots dr_n,$$

$$\Delta_n(s) \;=\; \int_0^1 \cdots \int_0^1 ((r_1 - q_1)^2 + \cdots + (r_n - q_n)^2)^{s/2}$$
$$dr_1 \cdots dr_n dq_1 \cdots dq_n.$$

As in the case of the $C_{n,k}$ considered here, a good starting point is provided by alternative integral representations for $\mathrm{R}s > 0$:

$$B_n(-s) = \frac{2}{\Gamma(s/2)} \int_0^\infty u^{s-1} b(u)^n \, du, \qquad b(u) = \frac{\sqrt{\pi}\mathrm{erf}(u)}{2u}$$

$$\Delta_n(-s) = \frac{2}{\Gamma(s/2)} \int_0^\infty u^{-s-1} d(u)^n \, du, \qquad d(u) = \frac{e^{-u^2} - 1 + \sqrt{\pi}u\,\mathrm{erf}(u)}{u^2}.$$

The first representation is given explicitly (see [27, equation (33)]), and the second one can be derived similarly. From the classic properties of the error functions, the functions $b(u)$ and $d(u)$ satisfy the linear differential equations

$$ub''(u) + 2(1 + u^2)b'(u) + 2ub(u) = 0,$$
$$2u^2 d'''(u) + 4u(3 + u^2)d''(u) + 4(3 + 4u^2)d'(u) + 8ud(u) = 0.$$

This is exactly the set-up of our Proposition 7.0. We thus deduce the existence of linear difference equations (with respect to s) for both B_n and Δ_n. The fast computation of the difference equation for B_n follows directly from the algorithm of the previous section, and, for instance, we get

$$(s + 9)(s + 10)(s + 11)(s + 12)B_4(s + 8)$$
$$-10(s + 8)^2(s + 9)(s + 10)B_4(s + 6)$$
$$+(s + 6)(s + 8)(35s^2 + 500s + 1792)B_4(s + 4)$$
$$-2(25s + 148)(s + 4)(s + 6)^2 B_4(s + 2)$$
$$+24(s + 2)(s + 4)^2(s + 6)B_4(s) = 0.$$

The recurrence holds for all s by meromorphic continuation. A result on the shape of this recurrence for arbitrary n could be obtained along the lines of Lemma 7.0.

7.3 Euler and Boole Summation Revisited

We explore a class of polynomials investigated recently by Borwein, Calkin and Manna [70]. The classic *Euler-Maclaurin summation* formula (see [1, entry 23.1.30] and [222, entry 2.11.1])

$$\sum_{j=a}^{n-1} f(j) = \int_a^n f(x) \, dx + \sum_{k=1}^m \frac{B_k}{k!} \left(f^{(k-1)}(n) - f^{(k-1)}(a) \right)$$
$$+ \frac{(-1)^{m+1}}{m!} \int_a^n \widetilde{B}_m(y) \, f^{(m)}(y) \, dy, \tag{7.35}$$

connects the finite sum of values of a function f, whose first m derivatives
are absolutely integrable on $[a, n]$, and its integral, for $a, m, n \in \mathbb{N}, a <$
n. Often it appears in introductory texts [6, 275], usually with mention
to a particular application—Stirling's asymptotic formula. In (7.35), the
B_l are the Bernoulli numbers and the $\widetilde{B}_l(x)$ are the periodic Bernoulli
polynomials. The *Bernoulli polynomials* are most succinctly characterized
by a generating function [1, entry 23.1.1]:

$$\frac{te^{xt}}{e^t - 1} \quad = \quad \sum_{n=0}^{\infty} B_n(x) \frac{t^n}{n!}. \tag{7.36}$$

The *periodic Bernoulli polynomials* are defined by taking the fractional
part of x: $\widetilde{B}_n(x) := B_n(\{x\})$ [222, entries 24.2.11–12]. Evaluation at the
point $x = 0$ gives the *Bernoulli numbers* [1, entry 23.1.2]: $B_l := B_l(0)$.

A similar formula starts with a different set of polynomials. The *Euler
polynomials* $E_n(x)$ are given by the generating function [1, entry 23.1.1]

$$\frac{2e^{xt}}{e^t + 1} \quad = \quad \sum_{n=0}^{\infty} E_n(x) \frac{t^n}{n!}. \tag{7.37}$$

Let the *periodic Euler polynomials* $\widetilde{E}_n(x)$ be defined by $\widetilde{E}_n(x+1) = -\widetilde{E}_n(x)$
and $\widetilde{E}_n(x) = E_n(x)$ for $0 \le x < 1$ [222, entries 24.2.11-12]. Now , define
the *Euler numbers* by $E_n := 2^n E_n(1/2)$ (see [1, entry 23.1.2] and [222,
entry 24.2.6])

$$\frac{2e^t}{e^{2t} + 1} \quad = \quad \sum_{n=0}^{\infty} E_n \frac{t^n}{n!}.$$

The alternating version of (7.35), using Euler polynomials, is the *Boole
summation* formula [222, entries 24.17.1–2]: Let $a, m, n \in \mathbb{N}, a < n$. If
$f(t)$ is a function on $t \in [a, n]$ with m continuous absolutely integrable
derivatives, then for $0 < h < 1$,

$$\sum_{j=a}^{n-1} (-1)^j f(j+h) \quad = \quad \frac{1}{2} \sum_{k=0}^{m-1} \frac{E_k(h)}{k!} \left((-1)^{n-1} f^{(k)}(n) + (-1)^a f^{(k)}(a) \right)$$

$$+ \frac{1}{2(m-1)!} \int_a^n f^{(m)}(x) \widetilde{E}_{m-1}(h-x) \, dx. \tag{7.38}$$

The first appearance is due to Boole [56]; but a similar formula is believed
to have been known to Euler ([220]). Mention of this elegant formula
in the literature is regrettably scarce, although in Borwein, Borwein, and

Dilcher [69, Section 2.2] it is used to explain a curious property of truncated *alternating* series for π and $\log 2$—for which Boole summation is better suited than Euler-Maclaurin.

In a 1960 note, Strodt [267] indicated a unified operator-theoretic approach to proving both of these formulae, but with very few of the details given. We aim, by following Borwein, Calkin, and Manna's work [70], to look at some of the details and the power of the approach.

7.3.1   Strodt's Operators and Polynomials

We introduce a class of operators on functions of a finite real interval. Let $C[\mathbb{R}]$ denote the continuous functions on the real line, in the supremum norm. Define, for $n \in \mathbb{N}$, the *uniform interpolation Strodt operators* $\mathcal{S}_n : C[\mathbb{R}] \mapsto C[\mathbb{R}]$ by

$$\mathcal{S}_n(f)(x) \quad := \quad \sum_{j=0}^{n} \frac{1}{n-1} \cdot f\left(x + \frac{j}{n-1}\right). \tag{7.39}$$

Since the operators defined by (7.39) are positive, they are necessarily bounded linear operators. We will show that an operator in this class sends a polynomial in x to another of the same degree. Furthermore, we obtain automorphisms on the ring of degree-k polynomials.

Proposition 7.74. *For each $k \in \mathbb{N}$, let $P_k := \{\sum_{i=0}^{k} a_i x^i : a_i \in \mathbb{R}\} \cong \mathbb{R}^{k+1}$. For all $n \in \mathbb{N}$, and $A \in P_k$ there is a unique $B \in P_k$, such that $\mathcal{S}_n(B) = A$.*

More broadly, define the generalized *Strodt operators*

$$\mathcal{S}_\mu(f)(x) \quad := \quad \int f(x+u)\, d\mu, \tag{7.40}$$

where the integral is Lebesgue on $\mathbb{R}$ and μ is a Borel probability measure. We can identify $\mathcal{S}_\mu$ and $\mathcal{S}_g(f)$ with the Lebesgue-Stieltjes integral $\int f(x+u)\, dG$ where $dG = g(u)\, du$ (see [269, pp. 282–284]). Thus, the original class $\{\mathcal{S}_n, n \in \mathbb{N}\}$ is covered by this definition. We continue to denote this class as $\mathcal{S}_g$. Now suppose $f \in P_k$; that is, $f := \sum_{n=0}^{k} f_n x^n$, for $f_n \in \mathbb{R}$. Then,

$$h(x) \quad := \quad \mathcal{S}_g(f) \;=\; \int \sum_{n=0}^{k} f_n(x+u)^n g(u)\, du.$$

The binomial theorem shows $h(x)$ is again a polynomial of degree k:

$$h(x) \quad = \quad \sum_{j=0}^{k} h_j x^j, \tag{7.41}$$

where $h_j = \sum_{n=j}^{k} f_n \binom{n}{j} M_{n-j}$ and

$$M_l \quad := \quad \int u^l \, dG(u). \tag{7.42}$$

We view the restriction of the operator $\mathcal{S}_g$ to $P_k \cong \mathbb{R}^{k+1}$ as a $(k+1)^2$ matrix. The coefficients of this matrix are:

$$\mathcal{S}_g\Big|_{P_k}[i,j] \quad := \quad \begin{cases} \binom{j-1}{i-1} M_{j-i} & \text{for } 1 \leq i \leq j \leq k+1 \\ 0 & \text{otherwise} \end{cases}. \tag{7.43}$$

Proposition 7.75. *Let g be a probability density function whose absolute moments exist. For all $h \in P_k$, there is a unique $f \in P_k$ so that $\mathcal{S}_g(f) = h$.*

Proof. From (7.43), $\mathcal{S}_g\Big|_{P_k}$ is an upper-triangular matrix with determinant

$$\det\left(\mathcal{S}_g\Big|_{P_k}\right) \quad = \quad \prod_{t=0}^{k} \binom{t}{t} X_{t,t} = 1,$$

and thus $h(x)$ is the unique solution of a linear system: $h = \mathcal{S}_g^{(-1)} f$.   □

Note that Proposition 7.0 follows as a special case. We recover both the Euler and Bernoulli polynomials by using different weight functions. Define the *Euler operator* as

$$\mathcal{S}_E(f)(x) \quad := \quad \frac{f(x) + f(x+1)}{2}; \tag{7.44}$$

i.e., $g(u) := \delta_0(u)/2 + \delta_1(u)/2$; and define the *Bernoulli operator* by

$$\mathcal{S}_B(f)(x) \quad := \quad \int_0^1 f(x+u) \, du; \tag{7.45}$$

i.e., $g(u) := \chi_{[0,1]}$. The Euler polynomials $E_n(x)$ form the unique solutions to

$$\mathcal{S}_E(E_n(x)) \quad = \quad x^n \quad \text{for all } n \in \mathbb{N}_0, \tag{7.46}$$

and the Bernoulli polynomials are the unique solutions to

$$\mathcal{S}_B(B_n(x)) \;\; = \;\; x^n \quad \text{for all } n \in \mathbb{N}_0. \tag{7.47}$$

Remark. This motivates introducing $\mathcal{S}_n$ in (7.39). The Euler operator is $\mathcal{S}_2$. The Bernoulli operator corresponds via a Riemann sum to the limit of $\mathcal{S}_n$ as $n \to \infty$. Hence, we provide an "interpolation" between these two developments.

   We shall prove that the generating functions of the Bernoulli and Euler polynomials follow from (7.46) and (7.47). This suggests a natural generalization which we will call *Strodt polynomials*, denoted as $P_n^g \equiv P_n, n \in \mathbb{N}_0$ (we typically suppress the g).

Theorem 7.76. *For each n in $\mathbb{N}_0$, let $P_n^g(x)$ be the Strodt polynomials associated with a given density $g(x)$; thus, $P_n^g(x)$ is defined by*

$$\mathcal{S}_g(P_n^g(x)) \;\; = \;\; x^n \quad \text{for all } n \in \mathbb{N}_0, \tag{7.48}$$

where $\mathcal{S}_g$ is a Strodt operator. Then

$$\frac{d}{dx}P_n^g(x) \;\; = \;\; nP_{n-1}^g(x) \quad \text{for all } n \in \mathbb{N}. \tag{7.49}$$

Proof. By the Lebesgue Dominated Convergence Theorem [248], we have that

$$
\begin{aligned}
\frac{d}{dx}\int P_n(x+u)g(u)du &= \lim_{\nu \to \infty}\int \nu\left(P_n(x+1/\nu+u) - P_n(x+u)\right)dG(u) \\
&= \int \lim_{\nu \to \infty}\nu\left(P_n(x+1/\nu+u) - P_n(x+u)\right)dG(u) \\
&= \int \frac{d}{dx}P_n(x+u)\,dG(u).
\end{aligned}
$$

Therefore, in view of (7.48), we have that

$$\mathcal{S}_g\left(\frac{d}{dx}P_n - nP_{n-1}\right) \;\; = \;\; \frac{d}{dx}(x^n) - nx^{n-1} = 0.$$

But $\mathcal{S}_g$ is one-to-one on polynomials by Proposition 7.0, hence the desired conclusion. □

   The Strodt polynomials comprise a subset of *Appell sequences* [246], polynomial sequences given by generating functions of the form

$$\sum_{n=0}^{\infty} A_n(x)\frac{x^n}{n!} = \frac{e^{xt}}{G(t)}.$$

Here $G(t)$ is defined formally by the coefficients of its series in t, where the leading term must not be zero. This is equivalent to (7.49) [246]. We next clarify the relation between Strodt and Appell.

Theorem 7.77. *Suppose a class of polynomials $\{C_n(x)\}_{n\geq 0}$ with real coefficients has an* exponential generating function

$$\sum_{n=0}^{\infty} C_n(x)\frac{t^n}{n!} \quad = \quad e^{xt}R(t), \tag{7.50}$$

with $R(t)$ continuous on the line. Then the exponential generating function of the image of the C_n under t, $\mathcal{S}_g$, is given by

$$\sum_{n=0}^{\infty} \mathcal{S}_g(C_n(x))\frac{t^n}{n!} \quad = \quad e^{xt}R(t)\,Q_g(t), \tag{7.51}$$

where

$$Q_g(t) \quad := \quad \int e^{ut}\,dG(u). \tag{7.52}$$

Proof. Assume t is within the radius of uniform convergence of (7.50) for an arbitrary value of x. Then we integrate (7.50) termwise to produce:

$$\sum_{n=0}^{\infty} \int C_n(x+u)\,g(u)\,du\,\frac{t^n}{n!} \quad = \quad \int e^{(x+u)t}R(t)\,g(u)\,du.$$

This is equivalent to (7.51).   □

As with $P_n^g(x) = P_n(x)$, the functions $Q_g(t) = Q(t)$ implicitly depend on the weight function $g(u)$.

Expanding the exponential integrand of (7.52) in a Taylor series, and then integrating termwise, we see that

$$Q(t) \quad = \quad \sum_{n=0}^{\infty} M_n\frac{t^n}{n},$$

where M_n is, as in (7.42), the nth moment of the cumulative distribution function of the density $g(u)$. Therefore $Q(t)$ is the *moment generating function* of g. Theorem 7.0 has the following consequence for the generating function of Strodt polynomials:

$$\sum_{n=0}^{\infty} P_n(x)\frac{t^n}{n!} \quad = \quad \frac{e^{xt}}{Q(t)}.$$

To see why, apply (7.51) with $C_n(x) = P_n(x)$, and conclude that $R(t)$ must equal $1/Q(t)$.

Now we see a precise connection: *the Appell sequence whose generating function comes in the form $e^{xt}/Q(t)$ is a Strodt polynomial sequence exactly when $Q(t)$ is the moment generating function of some cumulative distribution function.*

Corollary 7.78. *Formulae (7.46) and (7.47) are sufficient definitions of the classic Euler and Bernoulli polynomials, respectively.*

Proof. We show that the conditions (7.46) and (7.47) imply the generating function characterization of the two classes of polynomials. Start with the Euler polynomials, whose generating function is given by [222, entry 24.2.8]

$$\sum_{n=0}^{\infty} E_n(x)\frac{t^n}{n!} = \frac{2e^{xt}}{e^t + 1}. \tag{7.53}$$

The Euler polynomials satisfy

$$\sum_{n=0}^{\infty} \mathcal{S}_E(E_n(x))\frac{t^n}{n!} = \frac{2e^{xt}}{e^t + 1} \cdot Q_E(t) \tag{7.54}$$

by Theorem 7.0. We verify that

$$Q_E(t) = \int e^{ut}\left(\frac{\delta_0(u)}{2} + \frac{\delta_1(u)}{2}\right) du = \frac{e^t + 1}{2}, \tag{7.55}$$

and thus

$$\sum_{n=0}^{\infty} \mathcal{S}_E(E_n(x))\frac{t^n}{n!} = e^{xt} = \sum_{n=0}^{\infty} x^n \frac{t^n}{n!}. \tag{7.56}$$

Therefore, by uniqueness of power series coefficients, we have that for each integer $n \geq 0$, $E_n(x)$ is a polynomial of degree n that satisfies (7.46); that is,

$$\mathcal{S}_E(E_n(x)) = x^n \quad \text{for all } n \in \mathbb{N}_0. \tag{7.57}$$

Proposition 7.0 assures us that the $E_n(x)$ are completely determined by this property, so it can be used as a definition. The case for Bernoulli polynomials is similar; see Exercise 53. $\square$

7.3.2   A Few Consequences

Next, we explore some interesting special cases of Strodt polynomials and add to the list of properties that are directly implied by Theorems 7.0 and 7.0 (see [70] and Exercise 55 for much more on this issue).

   We first construct a binomial recurrence formula for Strodt polynomials that generalizes entry 23.1.7 in the *Handbook of Mathematical Functions* [1], which states that

$$B_n(x + h) \quad = \quad \sum_{k=0}^{n} \binom{n}{k} B_k(x) h^{n-k} \tag{7.58}$$

and

$$E_n(x + h) \quad = \quad \sum_{k=0}^{n} \binom{n}{k} E_k(x) h^{n-k}. \tag{7.59}$$

This property is another equivalent definition of Appell sequences [246].

Corollary 7.79. *For $n \in \mathbb{N}_0$, let $P_n(x)$ be a* Strodt polynomial *for a given weight function $g(u)$. Then*

$$P_n(x + h) \quad = \quad \sum_{k=0}^{n} \binom{n}{k} P_k(x) h^{n-k}. \tag{7.60}$$

Proof.   Since $\mathcal{S}_g(P_n(x)) = x^n$, it is not hard to show using the definition of $\mathcal{S}_g$ that

$$\mathcal{S}_g(P_n(x + h)) \quad = \quad (x + h)^n. \tag{7.61}$$

Use the binomial theorem to expand the right-hand side. Then each power x^k is equal to $\mathcal{S}_g(P_k(x))$, by definition. Thus, we have

$$\mathcal{S}_g(P_n(x + h)) \quad = \quad \mathcal{S}_g \left(\sum_{k=0}^{n} \binom{n}{k} P_k(x) h^{n-k} \right)$$

by the linearity of $\mathcal{S}_g$. Now apply $\mathcal{S}_g^{(-1)}$, invoking Proposition 7.0, to arrive at (7.60). $\square$

   The known recurrence formulae for Bernoulli and Euler polynomials can be derived directly from here; see Exercise 54.

7.3.3   Summation Formulae

Strodt's brief note [267] was intended to compare the summation formulae of Euler-Maclaurin and of Boole. We now explore a general formula and show how it can be specified to obtain both. We begin for a general density function. Let $z = a + h$ for $0 < h < 1$. For a fixed integer $m \geq 0$, define the *remainder* as

$$R_m(z) \quad := \quad f(z) - \sum_{k=0}^{m} \frac{\mathcal{S}_g(f^{(k)}(a))}{k!} P_k(h),$$

for a sufficiently smooth f. The process of deriving a summation formula in general effectively reduces to finding an expression for $R_m(z)$ as an integral involving the Strodt polynomials corresponding to the operator $\mathcal{S}_g$.

Start with $m = 0$. Since $P_0(z) = 1$ and $\int g(u) \, du = 1$, we have

$$R_0(z) \quad = \quad f(a + h) - \int f(a + u) \, g(u) \, du$$

$$= \quad \int [f(a + h) - f(a + u)] \, g(u) \, du \ .$$

We rewrite the integrand in the right-hand side as

$$f(a + h) - f(a + u) \quad = \quad \int_{u}^{h} f'(a + s) \, ds,$$

assuming f has a continuous derivative. By Fubini's theorem, we switch the order of integration, which yields

$$R_0(z) \quad = \quad \int \int_{u}^{h} f'(a + s) \, ds \, g(u) \, du \ = \ \int V(s, h) \, f'(a + s) \, ds,$$

where we define the piecewise function

$$V(s, h) \quad := \quad \begin{cases} \int_{-\infty}^{s} g(u) \, du & \text{for } s < h, \\ \int_{-\infty}^{s} g(u) \, du \ - \ 1 & \text{for } s \geq h. \end{cases} \ .$$

We now separate the Euler-Maclaurin and Boole cases.

(a) **Boole summation:** $P_n(x) = E_n(x)$ and $g(u) = (\delta(u) + \delta(u + 1))/2$. We calculate that

$$2 \cdot V(s, h) \quad = \quad \begin{cases} 1 & \text{for } 0 \leq s < h, \\ -1 & \text{for } h \leq s \leq 1, \\ 0 & \text{otherwise,} \end{cases} \ = \widetilde{E}_0(h - s)\chi_{[0,1]}(s),$$

where $\widetilde{E}_0(x)$ is the periodic Euler polynomial on $[0,1]$. Thus, we have

$$f(a+h) \quad = \quad \mathcal{S}_E(f(a)) + \frac{1}{2}\int_0^1 f'(a+s)\widetilde{E}_0(h-s)\ ds, \qquad (7.62)$$

which corresponds to (7.38) in the special case $m = 1$ and $n = a+1$.

We view this as the core formula in Boole summation; the rest of (7.38) is elaborated by summing and integrating by parts. We begin by rewriting (7.62) by using the change of variables $x := a+s$ in the integrand. Since $a \in \mathbb{N}$, $\widetilde{E}_0(a+h-s) = (-1)^a\widetilde{E}_0(h-s)$ and

$$f(a+h) \quad = \quad \frac{1}{2}(f(a) + f(a+1)) + \frac{(-1)^a}{2}\int_a^{a+1} f'(x)\widetilde{E}_0(h-x)\ dx.$$

Now take the alternating sum of both sides as j ranges from a to $n-1$. This telescopes, and we combine the intervals of integration to obtain a single integral on $[a, n]$. Hence,

$$\sum_{j=a}^{n-1}(-1)^j f(j+h) \quad = \quad \frac{1}{2}((-1)^a f(a) + (-1)^{n-1}f(n))$$

$$+\frac{1}{2}\int_a^n f'(x)\widetilde{E}_0(h-x)\ dx.$$

This is exactly (7.38) with $m = 1$.

To complete (7.38) for a general $m \geq 1$ requires induction. Integration by parts confirms that

$$\int_a^n f^{(k)}(x)\widetilde{E}_{k-1}(h-x)\ ds \quad = \quad \frac{\widetilde{E}_k(h)}{k}((-1)^{n-1}f^{(k)}(n) + (-1)^a f^{(k)}(a))$$

$$+\frac{1}{k}\int_a^n f^{(k+1)}\widetilde{E}_{k+1}(h-x)f^{(k+1)}(x)\ dx$$

for $k \geq 0$, which supplies the induction step.

(b) **Euler-Maclaurin summation** (see [267]): If we instead take $g(u) = \chi_{[0,1]}(u)$, then we write

$$V(s,h) \quad = \quad \begin{cases} s & \text{for } 0 \leq s < h, \\ s-1 & \text{for } h \leq s \leq 1, \\ 0 & \text{otherwise.} \end{cases} \quad .$$

Therefore,

$$R_1(z) \quad = \quad \int_0^1 V(s,h)f'(a+s)\ ds - \int_0^1 f'(a+s)\ ds\ \left(h - \frac{1}{2}\right)$$

$$= \quad \int_0^1 \widetilde{B}_1(s-h)\ f'(a+s)\ ds.$$

This needs the observation $V(s,h) - (h - 1/2) = \widetilde{B}_1(s-h)\, g(s)$. Hence,

$$f(a+h) = \int_0^1 f(s+a+h)\; ds + B_1(h)(f(a+1) - f(a))$$
$$+ \int_0^1 f'(a+s)\widetilde{B}_1(s-h)\; ds.$$

As for Boole, we are now essentially done. To recover (7.35), we simply integrate by parts and sum over consecutive integers. Summing over the integers within the interval $[a, n-1]$ yields

$$\sum_{j=a}^{n-1} f(j+h) = \int_a^n f(x+h)\; dx + B_1(h)(f(n) - f(a))$$
$$+ \int_a^n f'(x)\widetilde{B}_1(x-h)\; dx.$$

Here we have also shifted both interval integrations via $x := a + s$, giving the initial case for induction. Also,

$$\sum_{n=0}^{\infty} B_n(1-x)\frac{t^n}{n!} = \frac{te^{(1-x)t}}{e^t - 1} = \frac{te^{-xt}}{1 - e^{-t}} = \sum_{n=0}^{\infty} B_n(x)\frac{(-t)^n}{n!},$$

from which we derive by analytic continuation the well-known fact $\widetilde{B}_n(-h) = B_n(1-h) = (-1)^n B_n(h)$ for all $n \geq 0$ [1, entry 23.1.8]. Now integration by parts yields

$$\int_n^a f^{(k)}(x)\widetilde{B}_k(x-h)\; dx = \frac{(-1)^{k+1}B_{k+1}(h)}{k+1}\left(f^{(k)}(n) - f^{(k)}(a)\right)$$
$$-\frac{1}{k+1}\int_n^a f^{(k+1)}(x)\widetilde{B}_{k+1}(x)\; dx$$

for all $k \geq 1$, giving the induction step. The result is

$$\sum_{j=a}^{n-1} f(j+h) = \int_a^n f(x+h)\; dx + \sum_{k=1}^{m}\frac{B_k(h)}{k!}(f^{(k-1)}(n) - f^{(k-1)}(a))$$
$$+\frac{(-1)^{m+1}}{m!}\int_a^n f^{(m)}(x)\widetilde{B}_m(x-h)\; dx.$$

This is a generalized version of (7.35), as one can see as $h \to 0$.

(c) **Taylor series** approximation can be viewed as another case of this general approach. Let $g(u) = \delta(u)$, so that $\mathcal{S}_g(x^n) = x^n$. This means that

$P_n(x) = x^n$. We call this operator $\mathcal{S}_1$, to compare to (7.39) as well as to indicate that it is the *identity operator*. Now

$$V(s,h) \quad := \quad \begin{cases} 1 & \text{for } 0 < s < h, \\ 0 & \text{otherwise.} \end{cases} .$$

Thus,

$$f(a+h) \quad = \quad f(a) + \int_a^{a+h} f'(x) \, dx.$$

Again, use integration by parts to verify that

$$\int_a^{a+h} (x - a - h)^{k-1} f^{(k)}(x) \, dx \quad = \quad -\frac{(-h)^k}{k} f^{(k)}(a)$$
$$-\int_a^{a+h} (x - a - h)^k f^{(k+1)}(x) \, dx$$

for all $k \geq 1$. Therefore, by induction, for all $m \geq 0$,

$$f(a+h) \quad = \quad \sum_{k=0}^m f^{(k)}(a)\frac{h^k}{k!} + \frac{(-1)^m}{m!} \int_a^{a+h} (x - a - h)^m f^{(m+1)}(x) \, dx.$$

These derivations of Euler-Maclaurin and Boole summation formulae thus appear fully analogous to that of the Taylor series approximation. Lampret [200] has made this comparison in the Euler-Maclaurin and Taylor cases.

7.3.4   Asymptotic Properties

The NIST *Digital Library of Mathematical Functions* [222] presents asymptotic formulae for Bernoulli and Euler polynomials as $n \to \infty$. Specifically, [222, entries 24.11.5–6] give

$$(-1)^{\lfloor n/2 \rfloor - 1}\frac{(2\pi)^n}{2(n!)} B_n(x) \to \begin{cases} \cos(2\pi x), & n \text{ even}, \\ \sin(2\pi x), & n \text{ odd}, \end{cases} \qquad (7.63)$$

and

$$(-1)^{\lfloor (n+1)/2 \rfloor}\frac{\pi^{n+1}}{4(n!)} E_n(x) \to \begin{cases} \sin(\pi x), & n \text{ even}, \\ \cos(\pi x), & n \text{ odd}. \end{cases}$$

Convergence is uniform on compact subsets of $\mathbb{C}$.
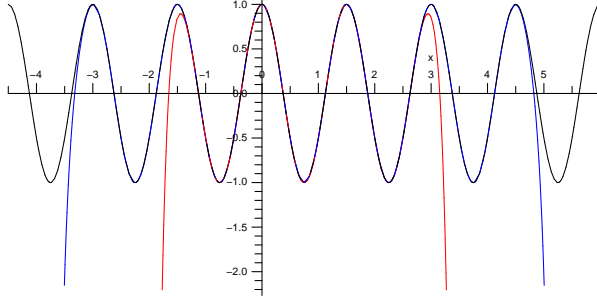
Figure 7.4. Graph of $\cos(4\pi/3)x$ versus $(-1)^{\lfloor n/2 \rfloor - 1} 2^{2n} \pi^{n+1}/(n! 3^{n+3/2}) P_n(x - 1/4)$ for $n = 20$ (light grey) and $n = 40$ (dark grey).

Experimenting with plots for real x as n becomes increasingly large suggests that a similar asymptotic property is true for any Strodt uniform interpolation polynomial $P_n(x)$.

As an example of our experimental results, Figure 7.4 displays the Strodt polynomials $P_n(x)$ for $g(u) = (\delta(u) + \delta(u - 1/2) + \delta(u - 1))/3$, which is the 3-point mean. We have displayed $n = 20$ and $n = 40$ for the Strodt polynomials, multiplied by a factor $(-1)^{\lfloor n/2 \rfloor - 1} 2^{2n} \pi^{n+1}/(n! 3^{n+3/2})$ and horizontally offset by $1/4$. They clearly appear to be converging to $\cos(4\pi x/3)$.

The general situation is this: *uniform Strodt polynomials* $P_n^m(x)$ on m points have the generating function

$$\sum_{n \geq 0} P_n^m(x) \frac{t^n}{n!} = \frac{m e^{xt}}{\sum_{j=0}^{m-1} \exp \frac{jt}{m-1}}. \qquad (7.64)$$

For $m = 2$, this generates the Euler polynomials. We used experimental evidence to formulate a conjecture for m-point asymptotics. Note that the the piecewise formulation above is unnecessary; for example, (7.63) could instead be written as

$$\frac{(2\pi)^n}{2(n!)} B_n(x) \sim \cos\left(2\pi x + \frac{n\pi}{2} + \pi\right).$$

This is the notation that we use here. It was quite easy to discover the offset, the period, the factorial, and the geometric terms in (7.66). Determining the constants C_m was more difficult. We set $x = 0$ and n even in

(7.66) and hunted for the minimal polynomial satisfied by C_m. We found values for $2 \le m \le 16$, and they appeared algebraic and to be simpler for m even. The first few polynomials—and associated radicals—plus some further numerical values suggested that the constants were trigonometric in origin. We then conjectured that $C_m \to 1/(2\pi)$ and that C_m was given by (7.65). Theorem 7.0 then followed with some work by using *Darboux's method* [227] to obtain the needed information from (7.64).

Theorem 7.80. *[70] For all $m \ge 2$, there are algebraic constants*

$$C_m \quad = \quad \frac{\csc\left(\frac{\pi}{m}\right)}{2m}. \qquad (7.65)$$

such that, as $n \to \infty$, we have uniformly in m and bounded x

$$C_m \frac{\pi^{(n+1)}}{n!} \left(\frac{2m-2}{m}\right)^n P_n^m(x) \quad \sim \quad \cos\left(\frac{2m-2}{m}\pi x + \frac{n\pi}{2}\right). \ (7.66)$$

For $m = 2$ and in the limit as $m \to \infty$ we recover known asymptotics for Euler and Bernoulli polynomials, respectively. The error in (7.66) is uniform; that is, it does not depend on m or x. This justifies our letting $m \to \infty$ to recover the asymptotic formulae for Bernoulli polynomials.

The reader is encouraged to plot various other cases of Theorem 7.0. There is not yet a conjecture for the precise asymptotic formula for general Strodt polynomials. Preliminary experiments suggest there will be similarly interesting and accessible results for continuous probability densities.

7.4   The QRS Oscillator Constant

The *Winfree model* of nonlinear physics describes a set of globally coupled phase oscillators (each individually exhibiting harmonics) with randomly distributed natural frequencies. The phenomenon of moving out of synchronization is called the unlocking transition. The oscillators described in this theory are quite general; they might even be bacteria. If there is sufficient interaction, the oscillators will tend to align. One of the many intriguing examples of coupled harmonic oscillation in nature is the fact, noted first on college campuses [215], that women living in close proximity tend to have synchronized menstrual cycles.

Quinn, Rand, and Strogatz, in a 2007 paper on coupled harmonics [237], utilized a summation describing a nonlinear Winfree-oscillator mean-field

system, namely

$$0 \quad = \quad \sum_{i-1}^{N} \left(2\sqrt{1 - s_N^2 \left(1 - 2\frac{i-1}{N-1} \right)^2} - \frac{1}{\sqrt{1 - s_N^2 \left(1 - 2\frac{i-1}{N-1} \right)^2}} \right),$$

(7.67)

where N represents the population size being considered in the model. In equation (7.67), s_N is an N-dependent variable that describes how far in or out of synchronization a group is, also called the phase offset. It can be written $s_N = \sin[\phi_0^*(1)]$, implicitly defining the angle $\phi_0^*(1)$, which measures how synchronized a group is in harmonic oscillation. For example, if we were to consider a system of two pendulums, $\phi_0^*(1)$ would represent how closely their swing patterns were aligned.

After computing values of s_N for various N, Quinn, Rand, and Strogatz [237] observed that

$$s_N \quad \sim \quad 1 - c_1 N^{-1}$$

for some constant $c_1 = 0.605443657\ldots$ (which we have now named as the *QRS constant*).

These authors wondered if this constant might be given in terms of some compact analytic formula, so they contacted the present authors and Richard Crandall. We did some additional analysis, leading to a resolution of this and some other constants. Portions of this section have been adapted from the resulting papers [29] and [132], which present full details.

We first attempted to compute this constant to higher numerical precision. Our computational approach was as follows. Hoping to obtain a numeric value accurate to at least 40 decimal digits, we employed the QD software, available from http://www.experimentalmath.info, which permits one to perform computations in a Fortran or C++ program to approximately 64-digit precision.

We rewrote the right-hand side of (7.67) by substituting $x = N(1-s)$, so that the roots of the resulting function $F_N(x)$ directly correspond to approximations to c_1. Given a particular value of N, we found the root of $F_N(x)$ by using iterative linear interpolation, in the spirit of Newton-Raphson iterations, until two successive values differed by no more than 10^{-52}. In this manner, we found a sequence of roots x_m for $N = 4^m$, where m ranged from 1 to 15. These successive roots were then extrapolated to the limit as $m \to \infty$ (or, in other words, as $N \to \infty$) by using *Richardson extrapolation* [258, p. 21–41], in the following form:

For each $m \geq 1$, set $A_{m,1} = x_m$. Then for $k = 2$ to $k = m$, successively set

$$A_{m,k} \;=\; \frac{2^k A_{m,k-1} - A_{m-1,k-1}}{2^k - 1}. \qquad (7.68)$$

This recursive scheme generates a triangular matrix A. The best estimates for the limit of x_m are the diagonal values $A_{m,m}$. Indeed, we found to our delight that for each successive m, the value $A_{m,m}$ agreed with $A_{m-1,m-1}$ to an additional three to four digits, which indicates that this extrapolation scheme is very effective for this problem.

In general, Richardson extrapolation employs a multiplier r where we have used 2 in the numerator and denominator of (7.68); the multiplier r depends on the nature of the sequence being extrapolated. We found that 2 is the optimal value to use here quite by accident—what we actually discovered is that $\sqrt{2}$ is the optimal multiplier when $N = 2^m$, which implies that 2 is optimal when $N = 4^m$. The resulting final extrapolated value $A_{15,15}$ obtained for $m = 15$ (corresponding to $N = 4^{15} = 1073741824$) is

$$c_1 \;\approx\; 0.60544365719673274947892284244720747522208996.$$

Since this and $A_{14,14}$ differed by only 10^{-38}, and successive values of $A_{m,m}$ had been agreeing to roughly four additional digits with each increase of m, we inferred that this numerical value was most likely good to 10^{-42}, or in other words to the precision shown, except possibly for the final digit.

We then attempted to recognize this numeric value by using the online Inverse Symbolic Calculator tool (*ISC2.0*) at `http://ddrive.cs.dal.ca/~isc`. Unfortunately, this tool was unable to determine any likely closed form.

So we explored other avenues. We began by defining, for $M = N - 1$,

$$\mathcal{P}_N(s) \;:=\; \sum_{k=0}^{M} \left(2\sqrt{1 - s^2(1 - 2k/M)^2} - \frac{1}{\sqrt{1 - s^2(1 - 2k/M)^2}} \right).$$

We then applied the *Poisson summation formula* [72, pp. 80–83], which for Lebesgue integrable functions $f(x)$ says that

$$\sum_{k=-\infty}^{\infty} f(k) \;=\; \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) e^{2\pi i n x} \, dx.$$

When the summation is truncated at finite limits, a related form is

$$\sum_{k=0}^{M} f(k) \;=\; \sum_{n=-\infty}^{\infty} \int_{-\eta}^{M+\eta} f(x) e^{2\pi i n x} \, dx,$$

provided $\eta \in (0,1)$. By setting $x = (M/2)(1 - (1/s)\cos t)$, we then derived

$$
\begin{aligned}
\mathcal{P}_N(s) &= \sum_{n=-\infty}^{\infty} \frac{M}{s} e^{i\pi nM} \int_0^\pi dt \, (1 - 2\sin^2 t) \, e^{-i\pi nM(\cos t)/s} \\
&= \frac{M}{s} \sum_{n=-\infty}^{\infty} e^{i\pi nM} \int_0^\pi \cos(2t) \, e^{-i\pi nM(\cos t)/s} \, dt \\
&= \frac{\pi M}{s} \sum_{n=1}^{\infty} (-1)^{nM} J_2\left(\frac{\pi nM}{s}\right),
\end{aligned}
$$

where J_2 is the standard Bessel function of order two.

This suggested to us that the sought-after zero s_N for the QRS problem is a solution to

$$
0 = \sum_{n=1}^{\infty} J_2\left(\frac{\pi nM}{s_N}\right) (-1)^{nM}.
$$

This we confirmed numerically for many small N. We noted that $J_2(z)$ can be written [1, p. 364] asymptotically as

$$
J_2(z) = \sqrt{\frac{2}{\pi z}} \left(\cos\left(z - \frac{5\pi}{4}\right) - \frac{15}{8z} \sin\left(z - \frac{5\pi}{4}\right) \right) + O\left(z^{-5/2}\right).
$$

This suggests that the Bessel function here is very close to a difference of the trigonometric functions shown (see Figure 7.5).

We then defined

$$
\begin{aligned}
\mathcal{Q}_s(z) &= \sum_{n=1}^{\infty} \frac{\cos(\pi nz - 5\pi/4)}{n^s} \\
&= -\frac{1}{\sqrt{2}} \left\{ \sum_{n=1}^{\infty} \frac{\cos(\pi nz)}{n^s} + \sum_{n=1}^{\infty} \frac{\sin(\pi nz)}{n^s} \right\} \\
&= -\frac{1}{\sqrt{2}} \left(\operatorname{Re} \operatorname{Li}_s\left(e^{i\pi z}\right) + \operatorname{Im} \operatorname{Li}_s\left(e^{i\pi z}\right) \right).
\end{aligned}
$$

Here $\operatorname{Li}_s(z) := \sum_{n=1}^{\infty} z^n/n^s$ (or its analytic continuation) is the *polylogarithm* we explored at length in *Experimentation in Mathematics* [72]. After significant additional manipulation, we were able to show that

$$
\mathcal{Q}_{1/2}(z) = -\frac{1}{\sqrt{2}} \zeta(1/2, z/2),
$$

where $\zeta(\cdot, \cdot)$ is the Hurwitz zeta function: $\zeta(s, a) = \sum_{n \geq 0}(n + a)^{-s}$. In summary, we concluded that c_1 is the unique zero in $(0, 2)$ of the function $\zeta(1/2, z/2)$.
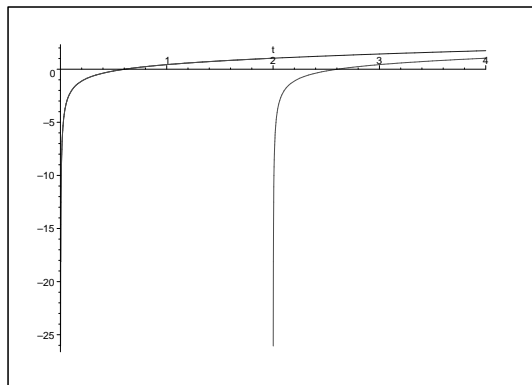
Figure 7.5.   The offset-periodic and Hurwitz zetas $\mathcal{Q}_{1/2}(z)$ and $-\zeta(1/2, z/2)/\sqrt{2}$, respectively (vertical) vs. z (horizontal) on $(0, 4)$. The $\mathcal{Q}_{1/2}$ function has a discontinuity at $z = 2$, to the left of which the two functions precisely coincide, are strictly monotone, and exhibit a zero $z_0 \approx 0.6$.

We emphasize, however, that the above derivation, which we have only briefly sketched here, when we first carried it out, was entirely conjectural and heuristic in nature. Indeed, a rigorous treatment (which was produced after the fact) occupies eight pages in the resulting paper [29]. But the fact that the end product of this derivation agreed to 42-digit accuracy with the numerical value we had earlier computed was compelling evidence that we were on the right track.

We continued this analysis, noting that most likely c_1 was merely the first coefficient of an asymptotic expansion

$$s_N = 1 - \frac{c_1}{N} + \frac{c_2}{N^2} - \frac{c_3}{N^3} \cdots .$$

After a similar process of computation and analysis, we found c_2 to be

$$c_2 = c_1 - c_1^2 - 30 \frac{\zeta(-\frac{1}{2}, \frac{1}{2}c_1)}{\zeta(\frac{3}{2}, \frac{1}{2}c_1)}.$$

Carrying this line of research further, Natalie Durgin (a student at Harvey Mudd College), Sofia Garcia (a student at Tulane University), and Tamara Flournoy (a student at the University of Michigan), together with one of the present authors (Bailey) wrote separate computer programs that, first of all, reproduced the numerical values c_1 and c_2 exactly (to the pre-

cision shown above), and then were able to calculate [132]

$$c_3 = 0.126314433612303666530616702052847758228073642787157869896$$
$$c_4 = -0.015937625178713939538299708463506509021108497772210531402.$$

The identity of these and higher-indexed constants is not known at this time, although it is conjectured that they have a flavor similar to c_2.

7.5 Proof Versus Trust

> ... that, in a few years, all great physical constants will have been approximately estimated, and that the only occupation which will be left to men of science will be to carry these measurements to another place of decimals.
>
> > – James Clerk Maxwell (1831-1879). Maxwell, who disagreed strongly with these views, was mocking them in his *Scientific Papers* 2, 244, October 1871.

In Section 1.3 of this book, we discussed the emerging experimental paradigm as it pertains to the acquisition of secure mathematical knowledge. This is an important enough question to merit some additional discussion. As before, we wish to emphasize that we are not suggesting that the traditional methods of formal proof be discarded. Nor do we offer any support to postmodern detractors who argue that mathematics and science are merely social constructs, with no claim to fundamental truth. Instead, we are more modestly asserting that the rapidly advancing computer technology of our era can be applied to a surprisingly wide range of modern mathematical problems, and that in some instances, at least, the impressive weight of empirical evidence must be taken seriously in support of key conjectures.

As one recent example of a proof in the classical sense, Benjamin Green and Terence Tao (the 2006 Fields Medalist) have just proved [155] that there are arbitrarily long arithmetic progressions of prime numbers (this was still a conjecture when the first edition of this book went to print). In other words, Green and Tao established that for every $n > 0$, there is a sequence of prime numbers $(p, p + d, p + 2d, \cdots, p + nd)$, for some integer d [155]. Their result is a *tour de force* of analytic number theory and other fields. But even here, it is interesting to note that the authors cite, as experimental evidence supporting this conjecture, a series of calculations searching for long arithmetic sequences of primes. The longest of these

computer-discovered sequences, of length 25, due to Raanan Chermoni and Jaroslaw Wroblewski, is $(6171054912832631 + 366384 \cdot 223092870 \cdot n,\ n = 0, 1, \cdots, 24)$ [291] (see also [72, Exercise 5, p. 254]).

Along this same line line, in his broad-ranging new book *The Proof Is in the Pudding*[1] Steven Krantz [191] writes

> So what will be considered a "proof" in the next century? There is every reason to believe that the traditional concept of pure mathematical proof will live on, and will be designated as such. But there will also be computer proofs, and proofs by way of physical experiment, and proofs by way of numerical calculation.

One real-world instance of this can be seen in the arena of primality testing, which we have discussed in some detail [72, Section 7.2]. If an integer of size at least 500 bits (roughly 167 digits) passes a single iteration of a well-known probabilistic primality test, then it is prime with "probability" at least $1 - 1/4^{28} \approx 1 - 7.2 \times 10^{-16}$. If an integer of this size passes six iterations, then the "probability" of false declaration is roughly one part in a googol. On the other hand, with the recently discovered Agrawal-Kayal-Saxena (AKS) primality test, one can formally certify primality without probabilistic testing [72, Section 7.2].

At the present time, the AKS-based tests have prohibitively high computational costs compared with the probabilistic tests. But even if these costs are greatly reduced through algorithmic improvements, one can still ask what is the AKS test's fundamental advantage, given that any real-world computer implementation of either of these schemes is subject to vagaries such as transcription errors, program bugs, system software errors and system hardware errors. The rate of hardware data integrity errors alone cannot be reduced much below about 10^{-18} in current computer technology. At this level (not to mention other more tangible sources of error), we submit that the distinction between a probabilistic test and a formal or "provable" test is moot.

True, the notion of "probability" in the above reckoning is a rather loose one; as a result, probability calculations of this sort can legitimately be questioned. But in spite of this and other issues that one might raise, banks, brokerages, and other large organizations have already voted with their pocketbooks—they use the probabilistic schemes, not the provable

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[1]In particular, we recommend [191, Chapter 8] with its substantial and up-to-date discussion of Perelman's work and Hales's recent results among other things. Contrary to what was anticipated in Exercise 7 of Chapter 1 of the first edition of this book, Hales's proof was ultimately published without an explicit disclaimer.

schemes, when generating large primes for secure communication, even for transactions involving millions of dollars (or pounds, euros or yen).

Along these same lines, whenever an experimental mathematician discovers a new mathematical identity (e.g., by using PSLQ) and verifies that it holds to very high precision, say 100 or more digits beyond the level that could reasonably be ascribed to round-off error (see Section 6.3), he or she must take such results very seriously.

The instructive examples that follow are but two of many that we could cite. Consider first this conjectured integral identity [25, Section 3.4]:

$$
\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \ln \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt \overset{?}{=} L_{-7}(2)
$$

$$
= \sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} \right.
$$
$$
\left. - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2} \right]. \tag{7.69}
$$

This result was found by one of the present authors (Borwein) and British physicist David Broadhurst. It arose from some studies in quantum field theory analyzing the volume of ideal tetrahedra in hyperbolic space, and is the simplest of 998 empirically determined cases in which the volume of a hyperbolic knot complement is expressible in terms of an L-series. The present authors tested this conjectured identity by computing the definite integral on the left-hand side to 20,000-digit precision by using a highly parallel implementation of the tanh-sinh quadrature algorithm (see [72, Section 7.4.3]; [25, Section 3.4.1]). Note that the integrand function has a nasty singularity within the interval of integration (see Figure 7.6). The right-hand side was evaluated to the same precision by using *Mathematica*. The results were identical, except for the final handful of digits.

For the second example, consider the following class of integrals that arise in the Ising theory of mathematical physics [28]:

$$
E_n := 2 \int_0^1 \cdots \int_0^1 \left(\prod_{n \geq k > j \geq 1} \frac{\frac{u_k}{u_j} - 1}{\frac{u_k}{u_j} + 1} \right)^2 dt_2 \, dt_3 \cdots dt_n.
$$

where $u_k := \prod_{i=1}^k t_i$. Along with Richard Crandall, we conjectured that

$$
E_5 \overset{?}{=} 42 - 1984 \operatorname{Li}_4 \left(\frac{1}{2} \right) + \frac{189\pi^4}{10} - 74\zeta(3) - 1272\zeta(3) \log 2 + 40\pi^2 \log^2 2
$$
$$
- \frac{62\pi^2}{3} + \frac{40\pi^2 \log 2}{3} + 88 \log^4 2 + 464 \log^2 2 - 40 \log 2. \tag{7.70}
$$
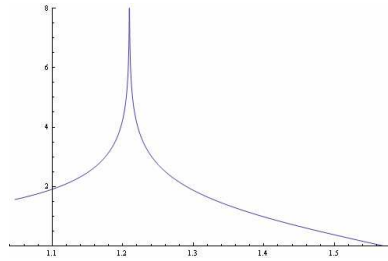
Figure 7.6. Singularity in the integrand function.

This evaluation was the end-product of a long series of difficult manipulations and high-precision quadrature. These manipulations reduced the above four-dimensional integral to the stultifying three-dimensional integral shown in Figure 7.7.

After this integral was evaluated numerically to 240-digit precision, PSLQ was employed to discover the evaluation given in (7.70). This evaluation is at least 190 digits beyond the level that could reasonably be ascribed to numerical round-off error. However, no formal proof is known.

Are such numerical discoveries, confirmed to hundreds or thousands of digits, merely chance? As with probabilistic primality tests, "probability" has at best a loose meaning in this context—we cannot define, in a rigorous manner, a measure space on a set such as the set of all computable reals because that set is only countably infinite, and in any event there are finite limits of the real computations we can perform given current technology. Also, we must acknowledge that in some exceptional cases, a high-level of numerical agreement does not certify that an apparent relation precisely holds [72, Section 1.4]. Perhaps the most remarkable example here is a class of sinc sums and integrals as described in Exercise 38. Some other examples are given in Exercises 51 and 66. But even in these cases, it is important to note that a reasonable rationale has been found for such behavior—it is not merely by capricious chance.

It is instructive to consider the reaction of the field of physics and cosmology to a similar coincidence, a paradox that has recently risen to a crisis level. The paradox derives from the fact that when one calculates, based on known principles of quantum mechanics, the "zero-point mass density" or the "vacuum energy density" of the universe, focusing for the time being on the electromagnetic force, one obtains the incredible result that empty space "weighs" 10^{93} grams per cc (the actual average mass density of the universe is 10^{-28} grams per cc) [270, p. 70–78]. Stephen

$$E_5 \;=\; \int_0^1 \int_0^1 \int_0^1 \Big[2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2$$

$$\big(-\big[4(x+1)(xy+1)\log(2)\,\big(y^5z^3x^7 - y^4z^2(4(y+1)z+3)x^6 - y^3z\,\big((y^2+1)\,z^2 + 4(y+$$

$$1)z+5\big)\,x^5 + y^2\,\big(4y(y+1)z^3 + 3\,\big(y^2+1\big)\,z^2 + 4(y+1)z-1\big)\,x^4 + y\,\big(z\,\big(z^2+4z$$

$$+5\big)\,y^2 + 4\,\big(z^2+1\big)\,y + 5z+4\big)\,x^3 + \big(\big(-3z^2-4z+1\big)\,y^2 - 4zy + 1\big)\,x^2 - (y(5z+4)$$

$$+4)x-1\big)\big/\big[(x-1)^3(xy-1)^3(xyz-1)^3\big] + \big[3(y-1)^2y^4(z-1)^2z^2(yz$$

$$-1)^2x^6 + 2y^3z\,\big(3(z-1)^2z^3y^5 + z^2\,\big(5z^3 + 3z^2 + 3z + 5\big)\,y^4 + (z-1)^2z$$

$$\big(5z^2 + 16z + 5\big)\,y^3 + \big(3z^5 + 3z^4 - 22z^3 - 22z^2 + 3z + 3\big)\,y^2 + 3\,\big(-2z^4 + z^3 + 2$$

$$z^2 + z - 2\big)\,y + 3z^3 + 5z^2 + 5z + 3\big)\,x^5 + y^2\,\big(7(z-1)^2z^4y^6 - 2z^3\,\big(z^3 + 15z^2$$

$$+15z+1\big)\,y^5 + 2z^2\,\big(-21z^4 + 6z^3 + 14z^2 + 6z - 21\big)\,y^4 - 2z\,\big(z^5 - 6z^4 - 27z^3$$

$$-27z^2 - 6z + 1\big)\,y^3 + \big(7z^6 - 30z^5 + 28z^4 + 54z^3 + 28z^2 - 30z + 7\big)\,y^2 - 2\,\big(7z^5$$

$$+15z^4 - 6z^3 - 6z^2 + 15z + 7\big)\,y + 7z^4 - 2z^3 - 42z^2 - 2z + 7\big)\,x^4 - 2y\,\big(z^3\,\big(z^3$$

$$-9z^2 - 9z + 1\big)\,y^6 + z^2\,\big(7z^4 - 14z^3 - 18z^2 - 14z + 7\big)\,y^5 + z\,\big(7z^5 + 14z^4 + 3$$

$$z^3 + 3z^2 + 14z + 7\big)\,y^4 + \big(z^6 - 14z^5 + 3z^4 + 84z^3 + 3z^2 - 14z + 1\big)\,y^3 - 3\,\big(3z^5$$

$$+6z^4 - z^3 - z^2 + 6z + 3\big)\,y^2 - \big(9z^4 + 14z^3 - 14z^2 + 14z + 9\big)\,y + z^3 + 7z^2 + 7z$$

$$+1\big)\,x^3 + \big(z^2\,\big(11z^4 + 6z^3 - 66z^2 + 6z + 11\big)\,y^6 + 2z\,\big(5z^5 + 13z^4 - 2z^3 - 2z^2$$

$$+13z+5\big)\,y^5 + \big(11z^6 + 26z^5 + 44z^4 - 66z^3 + 44z^2 + 26z + 11\big)\,y^4 + \big(6z^5 - 4$$

$$z^4 - 66z^3 - 66z^2 - 4z + 6\big)\,y^3 - 2\,\big(33z^4 + 2z^3 - 22z^2 + 2z + 33\big)\,y^2 + \big(6z^3 + 26$$

$$z^2 + 26z + 6\big)\,y + 11z^2 + 10z + 11\big)\,x^2 - 2\,\big(z^2\,\big(5z^3 + 3z^2 + 3z + 5\big)\,y^5 + z\,\big(22z^4$$

$$+5z^3 - 22z^2 + 5z + 22\big)\,y^4 + \big(5z^5 + 5z^4 - 26z^3 - 26z^2 + 5z + 5\big)\,y^3 + \big(3z^4 -$$

$$22z^3 - 26z^2 - 22z + 3\big)\,y^2 + \big(3z^3 + 5z^2 + 5z + 3\big)\,y + 5z^2 + 22z + 5\big)\,x + 15z^2 + 2z$$

$$+2y(z-1)^2(z+1) + 2y^3(z-1)^2z(z+1) + y^4z^2\,\big(15z^2 + 2z + 15\big) + y^2\,\big(15z^4$$

$$-2z^3 - 90z^2 - 2z + 15\big) + 15\big]\big/\big[(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2$$

$$(xyz-1)^2\big] - \big[4(x+1)(y+1)(yz+1)\,\big(-z^2y^4 + 4z(z+1)y^3 + \big(z^2+1\big)\,y^2$$

$$-4(z+1)y + 4x\,\big(y^2-1\big)\,\big(y^2z^2-1\big) + x^2\,\big(z^2y^4 - 4z(z+1)y^3 - \big(z^2+1\big)\,y^2$$

$$+4(z+1)y+1\big) - 1\big)\log(x+1)\big]\big/\big[(x-1)^3x(y-1)^3(yz-1)^3\big] - \big[4(y+1)(xy$$

$$+1)(z+1)\,\big(x^2\,\big(z^2 - 4z - 1\big)\,y^4 + 4x(x+1)\,\big(z^2-1\big)\,y^3 - \big(x^2+1\big)\,\big(z^2 - 4z - 1\big)$$

$$y^2 - 4(x+1)\,\big(z^2-1\big)\,y + z^2 - 4z - 1\big)\log(xy+1)\big]\big/\big[x(y-1)^3y(xy-1)^3(z-$$

$$1)^3\big] - \big[4(z+1)(yz+1)\,\big(x^3y^5z^7 + x^2y^4(4x(y+1)+5)z^6 - xy^3\,\big((y^2+$$

$$1)\,x^2 - 4(y+1)x - 3\big)\,z^5 - y^2\,\big(4y(y+1)x^3 + 5\,\big(y^2+1\big)\,x^2 + 4(y+1)x + 1\big)\,z^4 +$$

$$y\,\big(y^2x^3 - 4y(y+1)x^2 - 3\,\big(y^2+1\big)\,x - 4(y+1)\big)\,z^3 + \big(5x^2y^2 + y^2 + 4x(y+1)$$

$$y+1\big)\,z^2 + ((3x+4)y+4)z-1\big)\log(xyz+1)\big]\big/\big[xy(z-1)^3z(yz-1)^3(xyz-1)^3\big]\big)\big]$$

$$\big/\big[(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2\big]\; dx\,dy\,dz$$

Figure 7.7. Equivalent E_5 triple integral used for computer evaluation.

Hawking once quipped that this is the most spectacular failure of a physical theory in history [122, p. 147].

The "cosmological constant" of Einstein's general relativity equations is linearly related to the zero-point mass density. Einstein originally posited a nonzero value for the cosmological constant, but after the expansion of the universe was discovered, he lamented that this was his greatest blunder and set the constant to zero.

Physicists, who have fretted over the zero-point mass density paradox for decades, have noted that calculations such as the above involve only the electromagnetic force, and so perhaps when the contributions of the other known forces are included (bosons give rise to positive terms, whereas fermions give rise to negative terms), all terms will cancel out to exactly zero as a consequence of some unknown fundamental principle of physics. When "supersymmetry" was theorized in the 1970s, it was thought that it would meet this requirement, but when it was later discovered that our universe is not supersymmetric, this explanation was abandoned. In any event, until recently physicists remained hopeful that some yet-to-be-discovered principle would imply that the positive and negative terms of the zero-point mass density (and of the cosmological constant) precisely cancel out to zero.

These hopes were shattered with the recent discovery that the expansion of the universe is accelerating [288], which implies that the cosmological constant must be slightly positive. This "dark energy" also appears to be just what is needed to fill the 70% "missing mass" of the universe, which is needed to explain the observed fact that space is very nearly flat (i.e., Euclidean).

But this means that physicists are left to explain the startling fact that the positive and negative contributions to the cosmological constant cancel to 120-digit accuracy, yet fail to cancel beginning at the 121-st digit. Curiously, this observation is in accord with a prediction made by physicist Steven Weinberg in 1987, who argued from basic principles that the cosmological constant must be zero to within one part in 10^{120} or so, or else the universe either would have dispersed too fast for stars and galaxies to have formed, or else would have recollapsed upon itself long ago [270, p. 80–82].

At the same time, string theorists, who for 20 years have been earnestly seeking a complete and unique "theory of everything" that encompasses all known physical interactions, have instead deduced the existence of an enormous ensemble of possible universal laws, numbering (by one reckoning) more than 10^{500}. The vast majority of these universes are utterly hostile to any conceivable form of long-lived information-rich structure, much less life, and thus, if they truly exist somewhere, must be completely devoid of

observers. But with so many universes to choose from, some physicists now theorize, inevitably one (ours) beats the 1-in-10^{120} odds and is life-friendly. Needless to say, such "anthropic" reasoning constitutes a dramatic departure in philosophy from the traditional program of physics (and science in general), and many physicists are dead set against it.

In short, the recent discovery of the accelerating expansion of the universe and the implied slightly positive value of the cosmological constant constitutes, in the words of physicist Leonard Susskind, a "cataclysm," a "stunning reversal of fortunes" [270, p. 22, 154]. Some string theorists still hope that continuing work will lead to a resolution. David Gross, paraphrasing Winston Churchill, urges fellow theorists to "never, never, never give up" [270, p. 241]. But Lee Smolin, among others, argues that the discovery of the nonzero yet breathtakingly small cosmological constant, together with the derivation of 10^{500} universes when a single unique system was sought, constitutes a *reductio ad absurdum* of the entire string theory approach to modern physics, and we may need to start anew to formulate a coherent theory [263, p. 159].

However this debate turns out, it is worth emphasizing that everyone agrees that the cosmological constant coincidence, namely the fact that the component terms cancel to 120-digit accuracy, cannot merely be dismissed as a numerical curiosity. Indeed, the intensity of the current hand-wringing in the field is testament to the importance ascribed to this observation.

Similarly, we argue that results such as the two integral evaluations mentioned here, namely (7.69) and (7.70), even though they do not constitute rigorous proof, must be accepted as very compelling empirical evidence for these conjectured identities. Indeed, one can ask which is more firmly established: (1) a theorem proven at the end of a difficult 100+ page paper, which only a handful of colleagues other than the author has read, and which relies on dozens of other results by numerous other mathematicians spanning different fields of research; or (2) a conjectured identity, such as (7.69) above, for which no rigorous proof is known but which has been numerically verified to 20,000-digit accuracy?

More broadly, we observe from our experience working in this field that there appears to be little, if any, correlation between the difficulty of *discovering* a new relation or other fact and the difficulty of subsequently *proving* it. Indeed, there is no a priori reason why there should be any correlation.

Along this line, we should mention a recent result. Gregory Chaitin previously conjectured a "heuristic principle" that the theorems of a finitely specified theory cannot be significantly more complex than the theory itself, for a certain measure of complexity invariant under change of Gödel numbering. Recently, Calude and Jürgenson [100] succeeded in proving a

fairly strong form of this conjecture. In particular, they demonstrated that the theorems of a consistent and finitely specified theory that is arithmetically sound (e.g., Peano Arithmetic or ZFC) have bounded complexity (not the standard program-size complexity of Chaitin and Kolmogorov, but a computable variation of it). As a result, the fraction of true sentences of length n that are provable in the theory tends to zero when n tends to infinity [100].

Thus we are left to speculate whether the empirical methods for mathematical research that have been discussed in this volume and elsewhere might be seen as a tool to explore this realm of true but unprovable results, or even the realm of true but very-difficult-to-prove results. See, for instance, Exercise 68. At the least, such questions need some careful thought in a field that is destined, due to the unstoppable march of Moore's Law, to become ever more dependent on computational exploration. There is still time to probe these important questions.

7.6   Commentary and Additional Examples

1. **Radicals**. Find the minimal polynomials of

$$\sqrt{1+\sqrt{2}}, \sqrt{1+\sqrt{2+\sqrt{3}}}, \sqrt{\sqrt{1+\sqrt{2+\sqrt{3+\sqrt{4}}}}}$$

   by algebraic and by numeric methods. Conjecture a general form and verify it empirically.

   Hint: compute the radicals to high precision and use MinimalPolynomial or RootApproximant. The following is an algebraic method in *Maple* that takes the radical as input:

   ```
   r2p:=proc (A) global _X;
   sqrfree(evala(Norm(convert(_X-A,RootOf))),_X)[2][1][1] end;
   ```

   What is this code doing?

2. Find the closed form of the odd terms in Section 7.1.1.

3. **Changing bases**. For an integer k, characterize all pairs $x = a/(k-1), y = b/(k-1)$ such that $\{kx\} = y$ and $\{ky\} = x$. (Here $\{z\}$ denotes the fractional part of z.)
   Hint: look at the base-k representations of the (a, b) pairs.

4. **An integral of Oloa and Glasser** [286]. Determine the constants in

$$\frac{4}{\pi} \int_0^\pi \frac{y^2 \, dy}{y^2 + 4\ln^2(2\cos(\frac{y}{2}))} = a_1 + a_2\gamma + a_3\ln(2\pi). \qquad (7.71)$$

This integral evaluation, now proven, was discovered empirically.
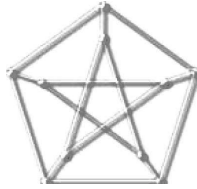
5.
Another example of emerging tools for mathematical experimentation is the Belgian project *GraPHedron* at `http://www.graphedron.net`, which offers "Automated and computer assisted conjectures in graph theory." The resource is easy to access and quite self-explanatory.

Abstract [216]: We present a new computer system, called GraPHedron, which uses a polyhedral approach to help the user to discover optimal conjectures in graph theory. We define what should be optimal conjectures and propose a formal framework allowing to identify them. Here, graphs with n nodes are viewed as points in the Euclidian space, whose coordinates are the values of a set of graph invariants. To the convex hull of these points corresponds a finite set of linear inequalities. These inequalities computed for a few values of n can be possibly generalized automatically or interactively. They serve as conjectures which can be considered as optimal by geometrical arguments. We describe how the system works, and all optimal relations between the diameter and the number of edges of connected graphs are given, as an illustration. Other applications and results are mentioned, and the forms of the conjectures that can be currently obtained with GraPHedron are characterized.

6. Identify
$$\mathcal{K} := \int_0^1 \frac{\left(-1 + 2t + t^2\right)\ln\left(1 - t\right)}{1 + 2t + 2t^2 - 2t^3 + t^4} \, dt$$

and hence develop a BBP formula (see Section 3.4]) for Catalan's constant.
Hint: You may find Prop. 3 in `http://www.pi314.net/hypergse6.php` helpful.

7. **A volume sum** [164]. Let V_n denote the volume of the unit Euclidean ball in n-dimensions, discussed in Section 5.4.1. Evaluate $\sum_{n=1}^\infty V_{2n}$ and $\sum_{n=1}^\infty V_{2n-1}$.
Hint: $\sum_{n=1}^\infty V_n = e^\pi \left(1 + \operatorname{erfc}(\pi^{1/2})\right) - 1$.

8. **A binomial identity**. Show, by two different methods, that for all positive integers n

$$\sum_{k=0}^{n} \binom{n}{k}\binom{2\,k}{k} = \sum_{k=0}^{n} \binom{n}{2\,k}\binom{2\,k}{k} 3^{n-2\,k}.$$

Compare $\sum_{k=0}^{\infty} \binom{n}{k}\binom{2\,k}{k}$ in *Maple* and in *Mathematica*.

9. **A problematic binomial identity**. In the *Monthly* Problem #11274 of February 2007, one is asked to show that

$$\sum_{k=0}^{m} 2^k \binom{2m-k}{m+n} = 4^m - \sum_{j=1}^{n} \binom{2m+1}{m+j} \qquad (7.72)$$

for $n, m \geq 0$. This problem is machine-solvable in both *Maple* and *Mathematica*. How easily, or even correctly, depends on who or what you know and which release you are using.

(a) Folkmar Bornemann [62], working in *Maple 9.5*, provided

```
> assume(n::natural,m::natural):
t1:=(m,n)->2^k*binomial(2*m-k,m+n):
t2:=(m,j)->binomial(2*m+1,m+j):
S:=(m,n)->sum(t1(m,n),k=0..m)+sum(t2(m,j),j=1..n):
```

We first show $S(m,n)$ independent of n. Indeed,

```
> simplify(sum(t1(m,n+1)-t1(m,n),k=0..m)+t2(m,n+1),
   GAMMA);
```

returns 0. We then evaluate $S(m,m)$ via

```
>  simplify(S(m,m));
```

which produces $S(m,m) = 4^m$ and completes the proof. As Doron Zeilberger points out, this works because *Maple* knows *Gosper's telescoping algorithm*.

(b) Try to derive identity (7.72) directly from Zeilberger's algorithm and to obtain the same recurrence for both sides.

(c) In early enough versions of *Maple*, using EKHAD (downloadable from `http://www.math.temple.edu/~zeilberg/programs.html`, with "rf" defined to be the rising factorial, you get

```
> zeil((2*m-k+1)*rf(1,r)*rf(-k,r)/rf(-2*m,r)/r!*2^r,
  r,m,M)[1];
  -2 (k - 2 m - 2) (k - 2 m - 3) + (m + 1) (2 m + 1) M
 > zeil((2*m+1)*rf(1,r)*rf(-k,r)/rf(2*m-k+2,r)/r!*(-1)^r,
  r,m,M)[1];
  -2 (k - 2 m - 2) (k - 2 m - 3) + (m + 1) (2 m + 1) M
```

Since the two expressions—equivalent to those in (7.72)—satisfy the same recurrence and initial conditions, they are equal.

(d) The same problem can be solved rather simply in *Mathematica* after loading the "fastZeil" package, which, along with numerous other useful software tools, is available from the website `http://www.risc.uni-linz.ac.at/research/combinat/software`. If you enter

```
Zb[2^k Binomial[2 m - k, m + n], {k, 0, m}, n]
Zb[Binomial[2 m + 1, m + j], {j, 1, n}, n]
```

and then perform FullSimplify on the difference of the two resulting expressions, the result is

$$\frac{2^{1-m}\Gamma(1+m)}{\Gamma(-n)\Gamma(2+m+n)},$$

which, since n is a nonnegative integer (and thus $\Gamma(-n)$ is a pole), is always zero.

10. **When limits matter**. Actually in Exercise 9, both *Maple10* and *Maple11* return $S(m,m) = 3 \cdot 4^m$. Indeed, even

```
> S(1,1)=simplify((subs(m=1,S(m,m))),GAMMA);
```

tells one that $4 = 12$. So our advice in Section 7.1.4 and the mantra of the second subsection ("A further caveat") to case-check was not made flippantly. The unsimplified command returns

$$2^{2\,m+1} + \frac{\binom{2\,m+1}{m+1}\Gamma\,(2+m)\,\sqrt{\pi}}{2\,\Gamma\,\left(m + \frac{3}{2}\right)}, \tag{7.73}$$

which hints at the cause of the difficulty—the package called some subroutines that converted combinatorics into analysis without taking proper care.

11. **Further moment recursions** The sequence $\{t^k\}$ in the integral of Proposition 7.0 can be replaced by more general sequences of functions that satisfy both a linear recurrence in k and a linear differential

equation in t. Provided that proper analytic conditions are satisfied at the endpoints of the path, the same result will hold. This makes it possible to compute, for instance, recurrences for the Fourier coefficients with respect to various bases such as orthogonal polynomials, Bessel functions, etc.

The algorithm that applies in this case is called *creative telescoping* discovered by Zeilberger [293] and further automated by Chyzak [106, 105]. Again, the computation boils down to linear algebra in a suitably constructed finite-dimensional vector space.

12. **Vacuum-diagram integrals.** British quantum field theorist David Broadhurst [92] has recently studied the *vacuum-diagram* integrals for $n \geq 0$:

$$V(n, a, b) \quad := \quad \int_0^\infty x^{2n+1+b} K_0^a(x) K_0^{'b}(x) \, dx$$

and provides the recursion

$$2(n+1)V(n, a, b) + a\, V(n, a-1, b+1) + b\, V(n+1, a+1, b-1) = 0$$

which preserves $N := a + b > 0$ and allows one to reduce to V values with $ab = 0$. Note that $K_0^{'} = -K_1$. For $N = 5$ we have presumably three independent terms which he takes to be $V(0, 1, 4) = -1/5$ and the two values $c_{5,1} = V(0, 5, 0)$ and $c_{5,3} = V(1, 5, 0)$—which the current authors came upon for entirely mathematical reasons. Proposition 7.0 applies to $n \mapsto V(n, a, b)$ for each a and b and as in Section 7.2.3 leads to very efficient code for the recursion.

13. **Realistic snowfakes**. Recent work on snowflake growth by Gravner and Griffeath is visible at `http://psoup.math.wisc.edu/Snowfakes.htm`. Papers, code and movies are offered. They are able to use appropriate automata (involving 'coupled lattice maps') to provide a taxonomy for increasingly realistic snowflakes whose formation pattern is also increasingly realistic, see figure to the right.

14. **Two recent *Monthly* integrals**. Identify the values of the two integrals from numerical calculation and then try to symbolically obtain the result.

   (a) (#11277, March 2007)

$$I_1 \quad := \quad \int_0^{\pi 2} \int_0^{\pi 2} \frac{\ln\left(2 - \sin s \cos t\right) \sin s}{2 - 2 \sin s \cos t + \sin^2 s \cos^2 t} \, ds \, dt.$$

(b) (#11275, February 2007)

$$I_2 \quad := \quad \int_0^\infty \int_y^\infty \frac{(x-y)^2 \ln\left[(x+y)/(x-y)\right]}{xy \sinh(x+y)} \, dx \, dy.$$

Hint: $I_1 \simeq .42756802899107$, and $I_2 \simeq 1.153265989080473$ reduces to a one dimensional integral on substituting $t = y/x$.

15. **A Fibonacci sum** [235]. Evaluate $\sum_{k=0}^{n-1} F_{n-k} 10^k$, where F_j is the j-th Fibonacci number.

16. **Correct the errors?** The following two rational pairs differ in only one coefficient. Which of

$$R_1 := \frac{26 + 5\,x^9 + 6\,x^7 + x^{16} + 7\,x^5 + x^{14} + x^{12}}{24 + 6\,x^9 + 8\,x^7 + 2\,x^{16} + 12\,x^5 + 3\,x^{14} + 4\,x^{12} + x^{21}}$$

or

$$R_2 := \frac{26 + 5\,x^9 + 6\,x^7 + x^{16} + 7\,x^5 + x^{14} + x^{12}}{24 + 6\,x^9 + 8\,x^7 + 2\,x^{16} + 16\,x^5 + 3\,x^{14} + 4\,x^{12} + x^{21}}.$$

is probably correct and why? Similarly, which of

$$R_3 :=$$

$$\frac{12\,x^2 + 7\,x^9 + 5\,x^{11} + x^{18} + 8\,x^3 + 4\,x^8 + 2\,x^{12} + x^{17} + x^{16} + 6\,x^4}{24 + 6\,x^9 + 8\,x^7 + 2\,x^{16} + 12\,x^5 + 3\,x^{14} + 4\,x^{12} + x^{21}}$$

or

$$R_4 :=$$

$$\frac{12\,x^2 + 7\,x^9 + 5\,x^{11} + x^{18} + 12\,x^3 + 4\,x^8 + 2\,x^{12} + x^{17} + x^{16} + 6\,x^4}{24 + 6\,x^9 + 8\,x^7 + 2\,x^{16} + 12\,x^5 + 3\,x^{14} + 4\,x^{12} + x^{21}}$$

is in error?

Hint: the coefficient 16 in R_2 is a typo.

17. **Four squares**. Prove that

$$(a^2 + b^2 + c^2 + d^2) \times (A^2 + B^2 + C^2 + D^2) \quad =$$
$$(aA + bB + cC + dD)^2 + (aB - bA + cD - dC)^2$$
$$+ (aC - bD - cA + dB)^2 + (aD - dA + bC - cB)^2.$$

This quaternion identity, which is easy to check symbolically, shows that it suffices to show every prime is the sum of four squares.

18. **π to thousands of digits from Vieta's formula**. Experiments
led Rick Kreminski [193] to the following formula generalizing that
of Vieta (see Exercise 21 of Chapter 5) for $n = 1, 2, \ldots$

$$\frac{\pi}{2} = 2^n \sin\left(\frac{\pi}{2^{n+1}}\right) + \sum_{m=1}^{\infty} \frac{k_m}{4^{nm}}$$

where $k_m := (-1)^{m+1}(\pi/2)^{2m+1}/(2m+1)!$. Confirm and then prove
this formula.

Now define $V_{0,n} := 2^n \sin\left(\pi/2^{n+1}\right)$ and recursively accelerate by

$$V_{k,n} = \frac{4^k V_{k-1,n+1} - V_{k-1,n}}{4^k - 1}.$$

Show that

$$|\pi - 2V_{k,n}| \leq 2C_k \, 10^{-6n(k+1)}$$

with

$$C_k := \prod_{j=1}^{k} \frac{1}{4^j - 1} \frac{\left(\frac{\pi}{2}\right)^{2k+3}}{(2k+3)!},$$

which decays very rapidly.

19. **A recreational Fibonacci continued fraction**. Posamentier and
Lehmann [235] record the following continued fraction introduced by
J. S. Madachy

$$\mu := 1 + \cfrac{1}{2 + \cfrac{3}{5 + \cfrac{8}{13 + \cfrac{21}{34 + \cfrac{55}{89 + \ldots}}}}} = 1.394186550228\ldots \qquad (7.74)$$

Compute substantially more digits of μ and attempt to discover a
closed form for it. None is known.

20. **Changing representations**. Compare e and π as decimals (they
both appear normal) and as continued fractions (See Figures 7.1.5
and 7.1.5).

(a) Does π appear to obey the *Gauss-Kuz'min* distribution: almost
all real numbers satisfy $\mathrm{Prob}(a_n = k) = -\log_2\left(1 - 1/(k+1)^2\right)$?
Here a_n is an entry in the simple continued fraction (see also Ex-
ercise 1 of Chapter 6).

(b) Attempt to discover the distribution experimentally by generating random continued fractions.

21. **A serious Fibonacci continued fraction** [280]. The rational number

$$\frac{19466773073171157536814300577691783136973102374888299968371004889104385}{1380349269358112757486951172455405090490221794434077311032504844759 8592}$$

is not remarkable but, in light of Exercise 20 above and Exercise 1 of Chapter 6, the fact that the first 40 terms of its continued fraction are

$$
\begin{bmatrix}
0 & 1 & 10 & 6 & 1 & 6 & 2 & 14 & 4 & 124 \\
2 & 1 & 2 & 2039 & 1 & 9 & 1 & 1 & 1 & 262111 \\
2 & 8 & 1 & 1 & 1 & 3 & 1 & 536870655 & 4 & 16 \\
3 & 1 & 3 & 7 & 1 & 140737488347135 & 8 & 128 & 2 & 1
\end{bmatrix}
$$

(read row by row) certainly is remarkable.

(a) Factoring the rational number above reveals the denominator is 2^{233} and the numerator has a 41-digit prime factor. Note that 233 is the 13th Fibonacci number. Confirm that the fraction is $\sum_{n=1}^{13} 2^{-F_n}$ with $F_1 = 1, F_2 = 2$ and $F_{n+1} = F_n + F_{n-1}$ again being the Fibonacci numbers.

(b) Compute the continued fraction of $\sum_{n=1}^{\infty} X^{-F_n}$ for a formal variable X. As pointed out by van der Poorten in [280], a generic continued fraction in $\mathbb{Q}(1/x)$ has mostly degree one entries and looks nothing like this.

(c) Experiment with other two-term recursions, starting with the Lucas numbers (Exercise 5 of Chapter 6).

This and much more is explained by van der Poorten in [280].

22. **Holte's amazing matrix**. For integer $b > 1$, Holte [172] studies the $m \times m$ matrix $\Pi_b(m)$ with (i, j) entry given by

$$(i, j, m, b) \mapsto b^{-m} \sum_{r=0}^{j} (-1)^r \binom{m+1}{r} \binom{m-1-i+(j+1-r)b}{m}$$

He shows that for a given b and m, this gives the transition probabilities $\Pi := \Pi_b^m = \{\pi_{i,j}\}$ for $0 \le i, j \le m-1$ of a finite (acyclic and irreducible) *Markov chain* for the probability of a "carry" in base-b

addition of m random n-digit random numbers. Thus, the probability of the $(k+1)$-carry being i given that the kth carry was i is independent of k and n. The core discoveries were made in *Mathematica*.

(a) Show by induction, or otherwise, that the maximum carry is
$$(m-1) - \lfloor (m-1)b^{-k} \rfloor$$

(b) Symbolically, discover and prove the closed form for the binary case:
$$\frac{1}{2} \begin{bmatrix} \frac{1+b}{b} & \frac{-1+b}{b} \\ \frac{-1+b}{b} & \frac{1+b}{b} \end{bmatrix}.$$

(c) Determine that the eigenvalues of Π_m^b are $(1, 1/b, \cdots 1/b^m)$ and the left eigenvectors of Π_b^m are independent of b.

23. **Unmasking a matrix**. In each of the following cases try to discover the structure of the given matrices. A fine source for matrix information is [52].

(a)
$$\begin{bmatrix} 2 & 3 \\ -1 & -2 \end{bmatrix} \begin{bmatrix} 2 & 1 & -2 \\ -1 & 1 & 6 \\ 0 & -1 & -3 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 5 \\ -1 & 1 & 0 & -10 \\ 0 & -1 & 1 & 10 \\ 0 & 0 & -1 & -4 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 1 & 1 & 1 & -4 \\ -1 & 1 & 0 & 0 & 15 \\ 0 & -1 & 1 & 0 & -20 \\ 0 & 0 & -1 & 1 & 15 \\ 0 & 0 & 0 & -1 & -5 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 1 & 1 & 7 \\ -1 & 1 & 0 & 0 & 0 & -21 \\ 0 & -1 & 1 & 0 & 0 & 35 \\ 0 & 0 & -1 & 1 & 0 & -35 \\ 0 & 0 & 0 & -1 & 1 & 21 \\ 0 & 0 & 0 & 0 & -1 & -6 \end{bmatrix}$$

(b) The matrix of left eigenvectors of $\Pi = \Pi_b^m$ of the previous exercise [172].

(c) The diagonalizing matrix in the representation $\Pi = V^{-1}DV$.

24. **Art, science and the circle problem**. Section 1.7 discusses Helaman Ferguson's mathematically inspired sculpture (see also [279]). Borwein, Bailey and Girgensohn explored *Madelung's constant* at

some length—along with its relation to sums of squares—in [72, Section 5.3]. The two have now been meshed in the sculpture shown in Figure 24 which is awarded bi-annually as the *David Borwein Distinguished Career Prize* of the Canadian Mathematical Society.

> This polished solid silicon bronze sculpture (2006) is inspired by the work of David Borwein, his sons and colleagues, on the conditional series for salt, Madelung's constant. This series can be summed to uncountably many constants; one is Madelung's constant for electro-chemical stability of sodium chloride." (Convexity is hidden here too!)

> This constant is a period of an elliptic curve, a real surface in four dimensions. There are uncountably many ways to imagine that surface in three dimensions; one has negative gaussian curvature and is the tangible form of this sculpture. (As described by the artist.)

The sum in question is

$$\mathcal{M}_3 = \sideset{}{'}\sum_{n,m,p} \frac{(-1)^{n+m+p}}{\sqrt{n^2+m^2+p^2}}$$

where the sum is taken over all nonzero integer triples.

Recent work on $r_2(n)$ [101] purports to show the spectacular resolution of the *circle problem*—the error in the average behavior of $r_2(n)$.

25. **Stirling's formula via the Poisson distribution**. In Section 5.5 we give an elementary proof of Stirling's approximation to $n!$. An attractive probabilistic approach is due to Mark Pinsky [230]. Via the Poisson distribution (see also Exercise 55b), Pinsky obtains

$$I_k \quad := \quad \frac{k^k}{k!} e^{-k} = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{k(e^{i\theta}-1-i\theta)} \, d\theta, \tag{7.75}$$

which can be symbolically evaluated (see also Exercise 26). Recall the Gaussian integral

$$J_k \quad := \quad \frac{1}{\sqrt{2\pi k}} = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-k\,\theta^2/2} \, d\theta \tag{7.76}$$

Figure 7.8. Madelung's constant in a Ferguson bronze

which is equivalent to $\Gamma(1/2) = \sqrt{\pi}$. To compare I_k and J_k write

$$I_k \;\; = \;\; \frac{1}{2\pi} \left(\int_{|\theta| \leq 1} + \int_{\pi \geq |\theta| \geq 1} \right) e^{k(e^{i\theta} - 1 - i\theta)} \, d\theta = I_k^{(1)} + I_k^{(2)}$$

$$J_k \;\; = \;\; \frac{1}{2\pi} \left(\int_{|\theta| \leq 1} + \int_{|\theta| \geq 1} \right) e^{-k\theta^2/2} \, d\theta = J_k^{(1)} + J_k^{(2)}.$$

(a) Estimate that $I_k^{(2)} \leq \exp(k(\cos 1 - 1))$ and

$$2\pi \, J_k^{(2)} \;\; \leq \;\; \int_{|\theta| \geq 1} |\theta| e^{-k\theta^2/2} d\theta = \frac{2}{k} e^{-k/2}.$$

Both tend to zero exponentially.

(b) Now estimate that

$$\left| I_k^{(1)} - J_k^{(1)} \right| \;\; \leq \;\; k \int_{-1}^{1} \frac{|\theta|^3}{3!} e^{-k\theta^2/3} \, d\theta = O\left(\frac{1}{k} \right), \qquad k \to \infty.$$

Hence $I_k - J_k = O(1/k)$, $k \to \infty$. But $J_k = 1/\sqrt{2\pi k}$, from which we reobtain Stirling's formula in the form

$$\lim_{k \to \infty} \sqrt{2\pi k} \, \frac{k^k}{k!} \, e^{-k} = 1$$

As discovered and proved in *Experimentation in Mathematics* [72, Section 1.5], we have $\sum_{k=1}^{\infty} \{J_k - I_k\} = 2/3 + \zeta(1/2)/\sqrt{2\pi}$. The proof relied on Lambert's W function; indeed, the nub of Pinsky's argument is variously in that literature.

26. **Evaluating the Poisson integral**. Evaluate the integral in (7.75). *Hint*: Make a change of variable $u := e^{ix}$ and compute the residue of $e^{ku} u^{-m-1}$ at zero.

27. **Dynamics of a sequence of digit sums** [235]. Consider the mapping $\sigma_2(m)$, which sends a positive integer m to the sum of the squares of its decimal digits:

$$m = \sum_{k=0}^{n} d_k 10^k \mapsto \sum_{k=0}^{n} d_k^2.$$

Show that in finitely many steps this dynamical system reaches the unique fixed point (one) or a unique period-eight cycle including the number four.
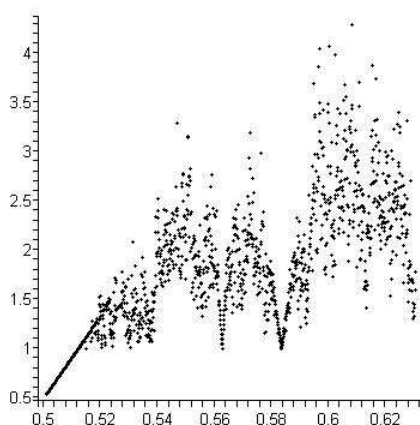
Figure 7.9. The function m on $[1/2, 2/3]$.

Consider $\sigma_p(m)$, which takes the pth power $(p = 2, 3, \ldots)$. Show that each such dynamical system in finitely many steps becomes periodic. What is the period structure?

Hint: for sufficiently large $n > n_p$, one has $n > \sigma_p(n)$. Estimate n_p and then computationally prove the assertion for $p = 2$.

28. **Dynamics of the mean-median map**. Starting with a finite set $S_n = \{x_1, \ldots, x_n\} \subset \mathbb{R}$, generate the unique number x_{n+1} which satisfies the *mean-median equation*:

$$\frac{x_1 + \cdots + x_n + x_{n+1}}{n+1} = \text{median}(S_n). \qquad (7.77)$$

As usual, we define the median of the set $S_n = \{x_1, \ldots, x_n\}$, where $x_1 \leq \cdots \leq x_n$, as

$$\text{median}(S_n) := \begin{cases} x_{(n+1)/2}, & n \text{ odd}, \\ \frac{x_{n/2} + x_{n/2+1}}{2}, & n \text{ even}. \end{cases} \qquad (7.78)$$

The set S_n is augmented to $S_{n+1} := S_n \cup \{x_{n+1}\}$. By applying the mean-median equation repeatedly to a set S_n, one generates an infinite sequence $\{x_k\}_{k=n+1}^{\infty}$. One may show that the limit of the medians of these sets is always monotone. Schultz and Shiflett [254] claim:

Strong Terminating Conjecture: *For every finite non-empty set $S \subset \mathrm{R}$, there exists an integer k such that the associated infinite sequence satisfies $x_j = x_k$ for all $j > k$. In other words, the sequence of new terms settles permanently to the median after a finite number of mean-median iterations.*

Chamberland and Martelli [104] made numerical investigations with *Maple* which suggest that the number of steps needed to settle down is unbounded. This leads to the weak terminating conjecture.

Weak Terminating Conjecture: *For every finite non-empty set $S \subset \mathrm{R}$, the limit of the medians is finite.*

The analysis with three initial points may be reduced to the canonical values $1/2 < x < 2/3$. Let $m : [0,1] \to \mathrm{R}$ represent the limit of the medians starting with $\{0, x, 1\}$, if the limit exists. Computer experimentation produces Figure 27. It is conjectured that m is continuous and affine almost everywhere.

Finally, can one determine the number of steps necessary to settle down corresponding to the affine segment connecting to $(1/2, 1/2)$?

29. **Random projections with noise**. The *method of random projections* [46] is a fundamental process in approximation and reconstruction problems. We consider a finite number n of closed convex sets C_k in Euclidean space (dimension more than one). We pick a starting point and take the Euclidean projection on one of the sets, say C_{k_1}, to be the next approximation:

$$x_1 \mapsto P_{C_{k_1}}(x_1) =: x_2 \mapsto P_{C_{k_2}}(x_2) := x_3 \mapsto \cdots \qquad (7.79)$$

Each set must be visited infinitely often. The method's behavior is not well understood if one has three or more sets whose intersection $\bigcap_{k=1}^{n} C_k$ is *empty*. This can happen in an iteration as numerical error and noise aggregate even if the sets ostensibly do intersect. We illustrate this in Figure 29 and note that we are recapturing a random Sierpinski triangle (see Section 2.1 as well as our chaos games in [25, §8.5]), where we have *under-relaxed* by moving only halfway to the set.

(a) Examine the algorithm in (7.79) when C_k is the kth side of a regular k-gon.

(b) Show that for two convex sets the method converges if and only if the minimal distance between the sets is attained; otherwise the iterates go to infinity.
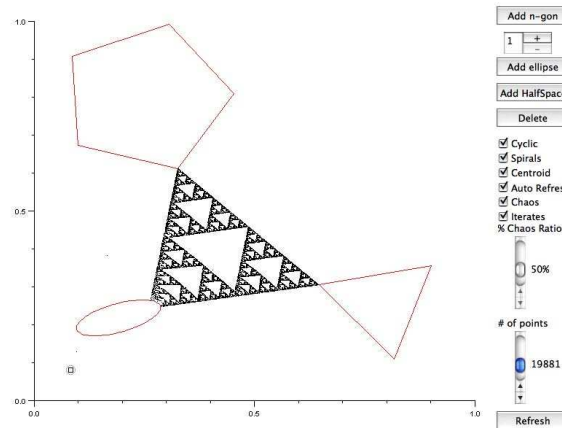
Figure 7.10. Sierpinski triangles

30. **Generalized harmonic binomial sums**. Let $H_a(n) = 1 + 2^{-a} + \cdots + n^{-a}$. Kalmykov, Ward, and Yost's Theorem A [180] states the following. For integer c the multiple (inverse) binomial sums

$$\sum_{j=1}^{\infty} \frac{1}{\binom{2j}{j}^{\pm 1}} \frac{z^j}{j^c} H_{a_1}(j-1) \cdots H_{a_p}(j-1)$$

are expressible in terms of Remiddi-Vermaseren functions, otherwise known as harmonic polylogarithms, which are special cases of certain multiple polylogarithms [25, p. 172].

31. **Desktop 3D**. Section 1.6 sketches the history of mathematical models. In late 2004, the *New York Times* printed a series of ten pictures of 19th century models photographed by Hiroshi Sugimoto to appear like monumental objects. In Figure 31 we juxtapose a plaster of Paris *Dini surface* beside a digital image reconstructed from the formula and used for manipulating and viewing in three dimensions on a stereo PC with polarized glasses. The photographer does not allow his images to be reproduced except in art books, but they may be viewed at `http://www.nytimes.com/slideshow/2004/12/02/magazine/\20041205_PORTFOLIO_SLIDESHOW` Note that we now actually have a surface not a solid—the virtual trumps the physical. Such a PC, as shown, costs only a few thousand dollars.

Figure 7.11. Nineteenth- and twenty-first century representations of the Dini surface.

32. **The error in** $\zeta(2)$**.** It is easy to show via summation by parts that

$$\zeta(2) \;=\; \sum_{n=1}^{\infty} \frac{H_n}{n(n+1)}, \tag{7.80}$$

where $H_n = \sum_{k=1}^{n} 1/k$ is the nth harmonic number. Show that for each positive integer p we have

$$\zeta(2) - \sum_{n=1}^{p-1} \frac{1}{n^2} \;=\; p! \sum_{n=1}^{\infty} \frac{H_n}{n(n+1)\cdots(n+p)}. \tag{7.81}$$

We note that

$$\sum_{n=0}^{\infty} \frac{1}{\binom{n+p+1}{p+1}} \;=\; \sum_{n=0}^{\infty} \frac{n!}{(p+2)\cdots(n+p+1)}$$

$$=\; {}_2\mathrm{F}_1 \left(\begin{array}{c} 1,1 \\ p+2 \end{array} \middle| 1 \right) = \frac{p+1}{p}$$

by Gauss's evaluation of a hypergeometric function at one (see [6, p. 66] and Exercise 47).

33. **Changing representations**. Let

$$a(q) := \sum_{m,n} q^{m^2+nm+n^2}, \, b(q) := \sum_{m,n} (\omega)^{n-m} q^{m^2+nm+n^2},$$

and

$$c(q) := \sum_{m,n} q^{(m+1/3)^2+(n+1/3)(m+1/3)+(n+1/3)^2},$$

where $\omega = e^{2i\pi/3}$. Then convince your self computationally that for $|q| < 1$ the functions a, b and c solve Fermat's equation [72, Exercise 14 of Chapter 4]: $a^3 = b^3 + c^3$. The neatest proof relies on expressing b and c as q-products. For example, $b(q)$ starts

$$(1-q)^3 \left(1-q^2\right)^3 \left(1-q^3\right)^2 \left(1-q^4\right)^3 \left(1-q^5\right)^3 \left(1-q^6\right)^2$$

$$\times \left(1-q^7\right)^3 \left(1-q^8\right)^3 \left(1-q^9\right)^2,$$

which tells us the closed form, whereas

$$a(q) \;=\; \frac{\left(1-q^2\right)^{21} \left(1-q^4\right)^{345} \left(1-q^6\right)^{8906} \left(1-q^8\right)^{250257}}{(1-q)^6 \left(1-q^3\right)^{76} \left(1-q^5\right)^{1734} \left(1-q^7\right)^{46662} \left(1-q^9\right)^{1365388}}$$

clearly has no such nice product. As sums, they look quite similar:

$$a(q) = 1 + 6\,q + 6\,q^3 + 6\,q^4 + 12\,q^7 + 6\,q^9 + 6\,q^{12} + 12\,q^{13} + 6\,q^{16}$$
$$+ 12\,q^{19} + O\left(q^{21}\right)$$

and

$$b(q) = 1 - 3\,q + 6\,q^3 - 3\,q^4 - 6\,q^7 + 6\,q^9 + 6\,q^{12} - 6\,q^{13} - 3\,q^{16}$$
$$- 6\,q^{19} + O\left(q^{21}\right).$$

Write code to replicate these results and to explore c.

34. **Khintchine's constant.** More than 10 years ago, in a paper on Khintchine's constant [26], we speculated that a certain explicitly defined constant satisfies the Khintchine property, namely that the geometric mean of the continued fraction terms converges to Khintchine's constant 2.68545... (see Exercise 2 of Chapter 6). It is known that "almost all" real numbers have this property, but it has been difficult to prove this property for any explicit real numbers.

Our constant was defined as follows. First, any for nonnegative integer n, we defined the *van der Corput sequence* to be the base-2 numbers $d_n = 0.b_0 b_1 b_2 \ldots$, where the b_i are the binary bits of n, with b_0 being least significant. The first few terms of the sequence d_n are

$$\left(\frac{1}{2}\right), \left(\frac{1}{4}, \frac{3}{4}\right), \left(\frac{1}{8}, \frac{5}{8}, \frac{3}{8}, \frac{7}{8}\right),$$
$$\left(\frac{1}{16}, \frac{9}{16}, \frac{5}{16}, \frac{13}{16}, \frac{3}{16}, \frac{11}{16}, \frac{7}{16}, \frac{15}{16}\right), \cdots$$

Next, we defined the sequence (a_n) as $a_0 := 0$, and

$$a_n := \lfloor \frac{1}{2^{d_n} - 1} \rfloor.$$

We then defined Z_2 to be the real number whose continued fraction terms are a_n, that is

$$Z_2 = [0; 2, 5, 1, 11, 1, 3, 1, 22, 2, 4, 1, 7, 1, 2, 1, 45, 2, 4, 1, 8, 1, 3, \cdots].$$

Our conjecture was that the geometric mean of the continued fraction expansion of Z_2 (i.e., the sequence (a_n)), is in fact the Khintchine constant K_0. We are pleased to report that this conjecture has now been proven by Thomas Wieting [287], thus providing a Champernowne-type continued fraction.

35. **Crossword pi.** On March 14, 2007, the *New York Times* ran a cross-word puzzle with a π theme (see Figure 7.12). To solve the puzzle, first note that the clue for 28 DOWN is "March 14, to Mathematicians," to which the answer is PIDAY. Moreover, roughly a dozen other characters in the puzzle are PI—for example, the clue for 5 DOWN was "More pleased" with the six character answer HAPπER. We include the completed puzzle on the following page (Figure 7.13).

36. **Integral proofs that** $355/113 > \pi$**.** We mention two recent integrals from [205] motivated by a discussion in *Experimentation in Mathematics* [72, Section 1.1], which showed

$$0 < \int_0^1 \frac{x^4(1-x)^4}{1+x^2}\, dx = \frac{22}{7} - \pi.$$

Indeed, the integral is an area and can be evaluated in closed form by most symbolic computation packages. The fact that $22/7$ is a convergent in the continued fraction for π seems largely be a coincidence; hence the growing complexity of the integrals below.

(a) Verify, and then prove, that

$$\frac{1}{3164} \int_0^1 \frac{x^8\left(1-x\right)^8\left(25+816\,x^2\right)}{1+x^2}\, dx \;=\; \frac{355}{113} - \pi,$$

and use this to prove that $355/113 - (7/2)\cdot 10^{-7} < \pi < 355/113 - (5/3 \cdot 10^{-7})$.

(b) Similarly, confirm

$$\int_0^1 \left\{\frac{x^{10}\left(1-x\right)^8}{4\left(1+x^2\right)} + \frac{5}{138450312}\right\} dx \;=\; \frac{355}{113} - \pi.$$

Hint: replace the upper limit in the integrals by $t > 0$.

37. **Geocaching and pi.** Geocaching is the name for a rapidly growing sport wherein participants armed with handheld Global Positioning System (GPS) receivers hunt for some of the 400,000 "geocaches" (typically small containers) hidden at latitude/longitude positions given on the website `http://www.geocaching.com`. Some of these require that a puzzle first be solved to obtain the geocache coordinates, and a surprising number of these puzzles involve computational mathematics. One example is the "Digits of Pi" geocache, located in vicinity of Berkeley, California, which presents this problem:

The New York Times Crossword

Edited by Will Shortz   No. 0314

Across
1 Enlighten
6 A couple CBS spinoffs
10 1972 Broadway musical
14 Metal giant
15 Evict
16 Area
17 Surface again, as a road
18 Pirate or Padre, briefly
19 Camera feature
20 Barracks artwork, perhaps
22 River to the Ligurian Sea
23 Keg necessity
24 "… ___ he drove out of sight"
25 ___ St. Louis, Ill.
27 Preen
29 Greek peak
33 Vice president after Hubert
36 Patient wife of Sir Geraint
38 Action to an ante
39 Gain ___
40 French artist Odilon ___
42 Grape for winemaking
43 Single-dish meal
45 Broad valley
46 See 21-Down
47 Artery inserts
49 Offspring
51 Mexican mouse catcher
53 Medical procedure, in brief
54 "Wheel of Fortune" option
57 Animal with striped legs
60 Editorial
63 It gets bigger at night
64 "Hold your horses!"
65 Idiots
66 Europe/Asia border river
67 Suffix with launder
68 Leaning
69 Brownback and Obama, e.g.: Abbr.
70 Rick with the 1976 #1 hit "Disco Duck"
71 Yegg's targets

Down
1 Mastodon trap
2 "Mefistofele" soprano
3 Misbehave
4 Pen
5 More pleased
6 Treated with disdain
7 Enterprise crewman
8 Rhone feeder
9 Many a webcast
10 Mushroom, for one
11 Unfortunate
12 Nevada's state tree
13 Disney fish
21 Colonial figure with 46-Across
26 Poker champion Ungar
27 Self-medicating excessively
28 March 14, to mathematicians
30 Book part
31 Powder, e.g.
32 007 and others: Abbr.
33 Drains
34 Stove feature
35 Feet per second, e.g.
37 Italian range
41 Prefix with surgery
44 Captain's announcement, for short
48 Tucked away
50 Stealthy fighters
52 Sedative
54 Letter feature
55 Jam
56 Settles in
57 Symphony or sonata
58 Japanese city bombed in W.W. II
59 Beelike
61 Evening, in ads
62 Religious artwork

Puzzle by Peter A. Collins

ANSWER TO PREVIOUS PUZZLE

A	R	F	S		A	C	H	E		O	R	G	A	N
C	O	R	K		T	R	E	X		K	E	R	R	Y
O	D	A	Y		L	A	I	T		S	T	A	T	S
L	E	N		R	A	N	D	O	M		I	P	S	E
D	O	C	T	O	R	K	I	L	D	A	R	E		
			R	A	G				S	I	E	S	T	A
T	Y	R	O	N	E	P	O	W	E	R		O	H	M
R	U	E	D			A	L	I			I	D	E	S
I	M	P		H	O	L	D	T	H	E	M	A	Y	O
B	A	A	B	A	A				O	R	E			
		I	R	I	S	H	C	O	U	N	T	I	E	S
P	E	R	I		T	I	R	A	D	E		D	X	C
A	R	M	E	D		T	A	T	I		Y	I	P	E
C	L	A	R	E		I	T	E	N		D	O	W	N

For answers, call 1-900-285-5656, $1.20 a minute; or, with a credit card, 1-800-814-5554.

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Figure 7.12. A PiDay crossword.

ANSWER TO PREVIOUS PUZZLE

Figure 7.13. Solution to the PiDay crossword.

The actual coordinates of the geocache are: North $37 + X$ degrees, West $122 + Y$ degrees, where X and Y are fractions between 0 and 1 defined as follows: Let $M = 8,468,347$, and let $N = 8,399,285$. Consider π expressed in hexadecimal (base-16) digits. Then X is the fraction after the "decimal" point has been shifted to the right by M places, and Y is the fraction after the "decimal" point has been shifted to the right by N places. Mathematically speaking, $X = \{16^M\pi\}$ and $Y = \{16^N\pi\}$, where $\{\cdot\}$ is fractional part.

Can you solve this to find the geocache coordinates? You need to calculate X and Y to at least five digit accuracy to locate the cache. As a check, the first two digits of X and Y (in decimal notation) are: $X = 0.88\ldots$, $Y = 0.24\ldots$.

Hint: use the BBP algorithm for π (see Section 3.4 and [20]).

38. **Some sinc sums.** Recall that $\operatorname{sinc}(x) := \sin(x)/x$. Motivated by the discussion of sinc integrals in Experimentation in Mathematics [72, Section 2.5], Robert Baillie was led to reexamine some earlier results on sinc sums [43]. Two of the most striking consequences follow.

   (a) Consider the following sum and integral involving $a := 1$ and

the reciprocals of odd primes.

$$\frac{1}{2} + \sum_{n=1}^{\infty} \operatorname{sinc}\left(\frac{n}{2}\right) \operatorname{sinc}\left(\frac{n}{3}\right) \operatorname{sinc}\left(\frac{n}{5}\right) \cdots \operatorname{sinc}\left(\frac{n}{23}\right) \operatorname{sinc}\left(\frac{n}{29}\right)$$

$$= \int_{0}^{\infty} \operatorname{sinc}\left(\frac{x}{2}\right) \operatorname{sinc}\left(\frac{x}{3}\right) \operatorname{sinc}\left(\frac{x}{5}\right) \cdots \operatorname{sinc}\left(\frac{x}{23}\right) \operatorname{sinc}\left(\frac{x}{29}\right) dx$$

$$= \pi \left(\frac{1}{2} - Q\right) \sim .499999990899\,\pi,$$

where Q is the rational number

$$\frac{3959735161333055430365082511104170654915014306538069299939389760351849}{435103498335938196749586681335393950889811560744584793771403209434374 8498175000},$$

as Baillie's conditions [43, Theorem 2] are satisfied. Similar integrals and sums stopping at primes before 29 equal $\pi/2$.

(b) Similarly, if we tweak the sequence very slightly by taking $a = 2$, giving the reciprocals of all the primes $\{p_k\}_{k=0}^{N}$ up to N, then we have the "sum plus $1/2$" and the integral equaling π only for the first two cases. For $N = 2$, Baillie's Theorem 2 [43] tells us each equals $\pi(1 - 1/240)$. However, the first equality in part (a) above (with the first term replacing 1 by $1/2$) holds until $\sum_{k=0}^{N} 1/p_k$ exceeds 2π [43, Theorem 1].

(c) We now estimate the N for which this occurs. The sum of the reciprocals of the primes diverges slowly. In fact, $\sum\{1/p \colon p \le x, p \text{ prime}\}$ is roughly $\log(\log(x)) + B$, where $B \sim 0.26149\ldots$ is the *Mertens constant* (see, e.g., [118, pp. 35, 79, 80]). In order for this sum to exceed 2π, x must be about $y = \exp(\exp(2\pi - B)) \sim 10^{179}$. Thus, by the Prime Number Theorem, $N \sim y/\log(y)$, which is about 10^{176}.

Thus, anyone who merely tested examples using these a_k would almost certainly *never* find an integer N for which the first equality above failed. Indeed, Crandall [120] proves the consequent error to be less than $10^{-10^{165}}$. Moreover, assuming the Riemann hypothesis, this upper bound reduces to $10^{-10^{178}}$, much less than one part in a googolplex. What is the metaphysical meaning of an error that small?

39. **More similar sinc sums.** Show for $N = 0, 1, 2, 3$, as observed by Baillie, that

$$\sum_{n=1}^{\infty} \frac{\sin(3n)}{3n} = \sum_{n=1}^{\infty} \left(\frac{\sin(n)}{n}\right)^{N} \frac{\sin(3n)}{3n}.$$

Hint: all four sums are $\pi/6 - 1/2$ [43, Theorem 1].

40. **Fun with Fourier series** [42]. Show that

(a)
$$\frac{\pi}{4} = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{2k-1} = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{2k-1} \operatorname{sinc}(2k-1),$$

(b)
$$\frac{\pi-1}{2} = \sum_{k=1}^{\infty} \frac{\sin(k)}{k} = \sum_{k=1}^{\infty} \frac{\sin^2(k)}{k^2},$$

(c)
$$\frac{\pi}{4} = \sum_{k=1}^{\infty} \frac{\sin^3(k)}{k} = \sum_{k=1}^{\infty} \frac{\sin^4(k)}{k^2},$$

(d)
$$\frac{3\pi}{16} = \sum_{k=1}^{\infty} \frac{\sin^5(k)}{k} = \sum_{k=1}^{\infty} \frac{\sin^6(k)}{k^2}.$$

(e) For $m = 0, 1, 2, 3$ but not for $m = 4$
$$\frac{\pi-3}{6} = \sum_{k=1}^{\infty} \operatorname{sinc}(3k) \operatorname{sinc}^m(k).$$

(f) For $m = 1, 2, 3$ but not for $m = 4$
$$\frac{\pi-2}{4} = \sum_{k=1}^{\infty} \cos(k) \operatorname{sinc}^m(k).$$

41. **Extensions of the Gauss-Wilson Theorem** One of the most remarkable results in elementary number theory is Wilson's theorem and its converse by Lagrange, stating that p is a prime if and only if

$$(p-1)! \equiv -1 \pmod{p}.$$

Less well known is a generalization due to Gauss, first mentioned in his *Disquisitiones*, §78. For the statement of this and related results it is convenient to let $N_n!$ denote the product of all integers up to N that are relatively prime to n, where N and n are positive integers. The theorem of Gauss can then be stated as follows:

$$(n-1)_n! \equiv \begin{cases} -1 \pmod{n} & \text{for } n = 2, 4, p^\alpha, \text{ or } 2p^\alpha, \\ 1 \pmod{n} & \text{otherwise,} \end{cases} \qquad (7.82)$$

for integers $n \geq 2$, where p is an odd prime and α is a positive integer. The first case of (7.82) indicates exactly those n that have primitive roots.

(a) A simple symmetry argument and Wilson's theorem yield

$$\left(\tfrac{p-1}{2}\right)!^2 \equiv (-1)^{\frac{p+1}{2}} \pmod{p},$$

an observation due to Lagrange (1773). This implies that the multiplicative order of $\left(\tfrac{p-1}{2}\right)!$ modulo p is 4 when $p \equiv 1 \pmod 4$, and is 1 or 2 otherwise; these last two cases were later completely determined by Mordell in 1961 by use of a class number condition.

(b) The question now arises whether there is a composite analogue to this characterization. This and related questions provide excellent examples for the power of the experimental approach. Based on numerous computations with *Maple*, Cosgrave and Dilcher [117] conjectured and then proved that, as before, only the orders 1, 2, and 4 can occur, and gave a complete characterization of all cases. The first and most important of these cases is actually true in a more general setting:

Let $M \geq 2$ and $n = p_1^{\alpha_1} \dots p_t^{\alpha_t}$, $t \geq 3$, with arbitrary positive exponents α_j. If $n \equiv 1 \pmod M$ and $p_j \equiv 1 \pmod M$ for at least three prime factors, then

$$\left(\tfrac{n-1}{M}\right)_n! \equiv 1 \pmod n. \tag{7.83}$$

For all odd n with at least three distinct prime divisors we then have

$$\left(\tfrac{n-1}{2}\right)_n! \equiv 1 \pmod n.$$

(c) Among the remaining few cases, the following is worth mentioning as fairly representative: Let $n = p^\alpha q^\beta$, where p and q are distinct odd primes with $p \equiv q \equiv 1 \pmod 4$, and α, β are positive integers. Then

$$\left(\frac{n-1}{2}\right)_n! \equiv \left(\tfrac{p}{q}\right) \pmod n,$$

where $\left(\tfrac{p}{q}\right)$ is the Legendre symbol which is 1 when p is a quadratic residue modulo q, and is -1 otherwise.

(d) The general result (7.83) indicates that one need not stop at the case of denominator $M = 2$. Indeed, some fascinating experimental results were obtained especially for $M = 3, 4$ and also for other M, partly proven, and partly only conjectured at this time [116]. Returning to the prime case, it was found experimentally, and subsequently proven, that $\frac{p-1}{4}! \equiv 1 \pmod{p}$ only for $p = 5$, while $(\frac{p-1}{4}!)^k \equiv -1 \pmod{p}$ for $k = 1, 2$, or 4 is impossible. However, the congruence

$$\left(\frac{p-1}{4}!\right)^8 \equiv -1 \pmod{p} \tag{7.84}$$

does hold for $p = 17, 241, 3361, 46817, 652081, \dots$ It turns out that (7.84) holds if and only if $p = a^2 + b^2$, where $a, b > 0$ and furthermore $p - 1 = 4ab$. This can be rewritten in terms of the Pell equation $(a - 2b)^2 - 3b^2 = 1$, and by the theory of Pell equations this sequence of primes can be obtained as follows: Define the sequences $\{x_k\}$, $\{y_k\}$ by $x_1 = 4$, $y_1 = 1$, and

$$x_k = 4x_{k-1} - y_{k-1}, y_k = x_{k-1}.$$

If $p_k = x_k^2 + y_k^2$ is a prime, then (and only then) it is a solution of (7.84). p_k is indeed prime for $k \leq 5$, but is composite for $6 \leq k \leq 1000$ except for seven primes corresponding to $k = 131$, $200, 296, 350, 519, 704$ and 950 (verified by Francois Morain); p_{950} has 1087 decimal digits.

Cosgrove and Dilcher [116] have experimentally obtained (and partially proven) similar results for other powers and for composite moduli.

42. **Symbolic residue computation.** Evaluate

$$\mathcal{I} \ := \ \int_0^\infty \frac{\text{sech}(t) \tanh(t)}{t} \, dt.$$

Hint: attempt symbolic residue computation in *Mathematica* or *Maple*. Try to identify I or I/π first.

43. **A more general ζ-formula**. For appropriate x and y,

$$\sum_{k=1}^{\infty} \frac{k}{k^4 - x^2 k^2 - y^4} = \frac{1}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k\binom{2k}{k}} \frac{5k^2 - x^2}{k^4 - x^2 k^2 - y^4} \prod_{m=1}^{k-1} \frac{(m^2 - x^2)^2 + 4y^4}{m^4 - x^2 m^2 - y^4}.$$

This bivariate generating function identity for odd ζ-values was empirically conjectured by Henri Cohen and proved independently by

Rivoal [244] and Bradley [24]. Is there a corresponding even ζ-formula?

44. Discover the closed form for

$$\int_0^1 t^n (1-t)^{n-1} P_n^{(n)} \left(1 - \frac{t}{2}\right) dt$$

and so obtain the value of (7.5) when $x = 1/2$.
Hint: the following *Maple* code may help:

```
with(orthopoly):
T:=(a,n)->int(t^(n)*(1-t)^(n-1)*GegenbauerC(n,n,1-2*t*a^2),
    t=0..1);
```

45. Use the Bohr-Mollerup theorem of Section 5.4 to prove the *triplication formula* for $\Gamma(x)$, namely that

$$2\pi\,\Gamma(3x) \;=\; 3^{3x-1/2}\,\Gamma(x)\,\Gamma\left(x + \frac{1}{3}\right)\,\Gamma\left(x + \frac{2}{3}\right).$$

This and the duplication theorem Example 13 of Chapter 5 to establish (7.4) and complete Grivaux's proof in Section 7.1.4.

46. Provide details for the proof of (7.9). Find the corresponding proof for (7.10).

47. Use (7.14) to deduce Gauss's evaluation

$$ {}_2F_1\left(\begin{array}{c} a,b \\ c,k \end{array} \middle| 1 \right) \;=\; \frac{\Gamma(c-a)\Gamma(c-b)}{\Gamma(c)}. \qquad (7.85)$$

48. Find a closed form for the Champernowne number λ discussed in Section 7.1.5 and Exercise 5 of Chapter 4. Do this correspondingly for each base b. Explore the continued fraction of the resulting λ_b.

49. Recall that the additive partition function is generated by the function $1/\prod_{k=1}^{\infty}(1-q^k)$ (see [72, Chapter 4] and [283, Section 5.2]). Reshape the first hundred coefficients modulo $5, 7$, and 11 to highlight Ramanujan's congruences [25, 72]. For example. for modulo 7

we have the 9×7 matrix

$$\begin{bmatrix}
1 & 2 & 3 & 5 & 0 & 4 & 1 \\
1 & 2 & 0 & 0 & 0 & 3 & 2 \\
1 & 0 & 3 & 0 & 0 & 4 & 1 \\
1 & 2 & 0 & 5 & 0 & 0 & 1 \\
1 & 4 & 3 & 5 & 0 & 4 & 1 \\
1 & 0 & 3 & 0 & 0 & 0 & 2 \\
2 & 2 & 3 & 5 & 0 & 0 & 2 \\
1 & 4 & 0 & 0 & 0 & 0 & 3 \\
2 & 2 & 3 & 5 & 0 & 4 & 2
\end{bmatrix}.$$

50. **The Prouhet-Tarry-Escott problem**, [82, Chapter 11], [72, Exercise 16 of Chapter 5]. Given positive integers n and k, one form of this problem is cast as a Diophantine equation seeking nontrivial solutions to

$$\begin{aligned}
\alpha_1 + \alpha_2 \cdots + \alpha_n &= \beta_1 + \beta_2 + \cdots \beta_n \\
\alpha_1^2 + \alpha_2^2 + \cdots + \alpha_n^2 &= \beta_1^2 + \beta_2^2 + \cdots \beta_n^2 \\
&\cdots \\
\alpha_1^k + \alpha_2^k + \cdots + \alpha_n^k &= \beta_1^k + \beta_2^k + \cdots \beta_n^k.
\end{aligned}$$

A solution is abbreviated as $[\alpha] =_k [\beta]$. For example,

$$[-2, -1, 3] =_2 [2, 1, -3], \qquad [-5, -1, 2, 6] =_3 [-4, -2, 4, 5]$$

$$[-8, -7, 1, 5, 9] =_4 [8, 7, -1, -5, -9],$$

and such *ideal solutions* with $k = n - 1$ are known for $n \leq 12$, except for $n = 11$.

David Broadhurst [92] has recently found a second inequivalent solution for $n = 12$, using the Chinese remainder theorem modulo 141 and 53 along with intensive and clever programming. It is

$$[\pm 472, \pm 639, \pm 1294 \pm 1514, \pm 1947, \pm 2037] =_{11} [\pm 257, \pm 891, \pm 1109, \\ \pm 1618, \pm 1896, \pm 2058]$$

since

$$\begin{aligned}
& 472^{2k} + 639^{2k} + 1294^{2k} + 1514^{2k} + 1947^{2k} + 2037^{2k} \\
= \; & 257^{2k} + 891^{2k} + 1109^{2k} + 1618^{2k} + 1896^{2k} + 2058^{2k}
\end{aligned}$$

for $k = 1, 2, \ldots, 5$. Until then only

$$[\pm 151, \pm 140, \pm 127, \pm 86, \pm 61, \pm 22] =_{11} [\pm 148, \pm 146, \pm 1271, \pm 94, \\ \pm 47, \pm 35]$$

discovered by Chen Shuwen in 1999 had been known. (Note that in *Experimentation in Mathematics* [72], the element ± 86 was mistranscribed as ± 186.)

51. **Some recent partition congruences.** Mahlburg [211] proved inter alia that for every prime $p > 3$ there are infinitely many pairs (A, B) such that $M(r, p, An + B) = 0 \pmod{p}$ for $r = 0, 1, \ldots, p - 1$. The result is entirely existential. Actually, Mahlburg proved the result for prime powers. Here $M(r, p, n)$ is the number of partitions of n with *crank* congruent to $r \bmod p$. The crank [8] of a partition is the largest part if the partition has no ones, otherwise it is the difference between the number of parts larger than the number of ones and the number of ones. Bringmann [89] has proved the rank-analog $N(r, p, An + B) \equiv 0 \pmod{p}$. Bringmann's result is also purely existential but also handled the case of prime powers. Earlier, Bringmann and Ono [91] proved the analogous result $N(r, p_1, An + B) \equiv 0 \pmod{p_2}$ when p_1 and p_2 are relatively prime. Here $N(r, p, n)$ is number of partitions of n with *rank* congruent to $r \bmod p$. Dyson [133] defined the rank of a partition as the largest part minus the number of parts. Recently, Garvan [142] found a different proof of the rank-analog $N(r, p, An + B) \equiv 0 \pmod{p}$ as well as some nontrivial examples. For example, for $r = 0, 1, \ldots, 10$,

$$N(r, 11, 54 \cdot 11 \cdot 194 \cdot n + 4322599) \equiv 0 \pmod{11} \qquad (1)$$

and

$$N(r, 11, 112 \cdot 194 \cdot n + 172904) \equiv 0 \pmod{11}. \qquad (2)$$

So far, Garvan has verified only (2) for $n = 0$ using Fortran (*Maple* has no hope of doing such a computation). For details, see Garvan's work [90, 142].

We mention this result, in part, as another example of a highly technical proof of an existential result which, while easy to understand, is very hard to verify.

52. **Pictures of Strodt polynomials**. The easy accessibility of plotting routines—now excellent, for example, in *Maple*, *Mathematica*, and MATLAB—should make graphing a ubiquitous part of mathematical
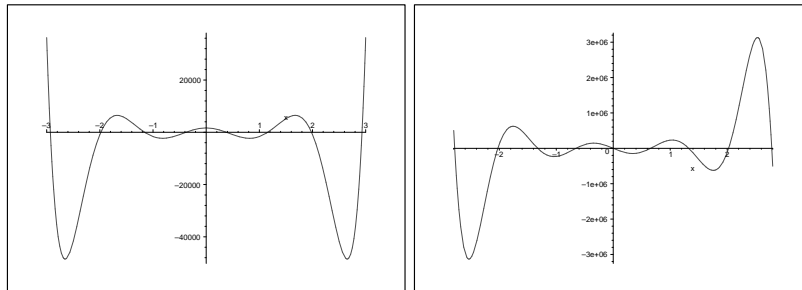
Figure 7.14. The Hermite polynomials for $n = 8$ (left) and $n = 11$ (right).
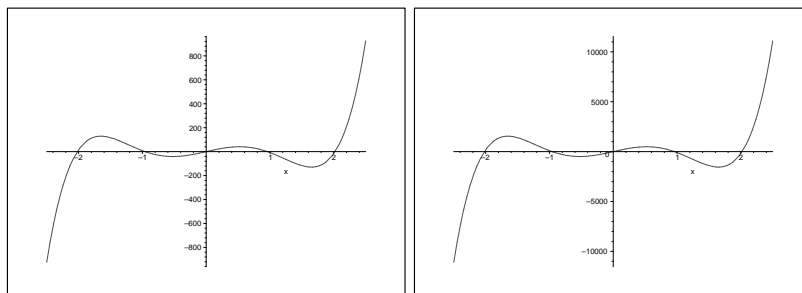
Figure 7.15. The Hermite polynomial for $n = 5$ (left) and the derivative for $n = 6$ (right).

life. It also partially explains why there relatively few pictures in the main text.

Thus, as we saw in Section 7.3, plotting plays a key part of both the research and preparation process. Figure 52 draws small values of Hermite polynomials. In deciding the domain and degrees one learns a great deal quickly. Also, as normalizations of orthogonal polynomials differ, it is a very good sanity check. Note that in each case we have trapped all the—necessarily real—roots and so the pictures are reliable. We also confirm the odd/even properties of the sequence.

53. Provide the proof of Corollary 7.0 for Bernoulli polynomials.

54. Use Corollary 7.0 to establish (7.59) and (7.58).

55. **Strodt polynomials of probability densities.** We consider three key examples here. In each case, we suggest making plots of the same character as in Exercise 52.

(a) **Gaussian density function**. We take $g(u) := \frac{1}{\sqrt{\pi}} e^{-u^2/2}$. The moment generating function is

$$Q(t) \;=\; \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{ut}\, e^{-u^2/2}\, du \;=\; e^{t^2/4}. \qquad (7.86)$$

The generating function for the Strodt polynomials is thus

$$\sum_{n=0}^{\infty} P_n(x) \frac{t^n}{n!} \;=\; \frac{e^{xt}}{Q(t)} \;=\; e^{xt - t^2/4}. \qquad (7.87)$$

Similarity to the *Hermite polynomials* is evident; their generating function is $e^{2xt - t^2}$ [1, entry 22.9.17]. Thus, the Strodt polynomials are scalings of the Hermite polynomials, as

$$2^n P_n(x) \;=\; H_n(x) \quad \text{for all } n \geq 0.$$

We have an immediate consequence to Theorem 7.0 and 7.0.

Proposition 7.81. *The Hermite polynomials $H_n(x)$ are scaled Strodt polynomials for the Gaussian density. They satisfy*

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} H_n(x + u)\, e^{-u^2/2}\, du \;=\; (2x)^n, \qquad (7.88)$$

and

$$\frac{d}{dx} H_n(x) \;=\; 2n H_{n-1}(x). \qquad (7.89)$$

Hermite polynomials form the only orthogonal Appell sequence [256], and so are the only orthogonal Strodt polynomials.

(b) **Poisson distribution**. The *Poisson distribution* X for a real parameter λ is given by the probability function

$$P(X = j) \;=\; e^{-\lambda} \frac{\lambda^j}{j!} \qquad \text{for } j \in \mathbb{N}_0. \qquad (7.90)$$

This corresponds to the weight function

$$g(u) \;:=\; \sum_{j=0}^{\infty} \delta_j(u) e^{-\lambda} \frac{\lambda^u}{\Gamma(u+1)}. \qquad (7.91)$$

We construct the Strodt polynomials for this distribution, using Theorem 7.0. Since the moment generating function is

$$Q(t) \;\; = \;\; e^{-\lambda} \sum_{j=0}^{\infty} e^{jt} \frac{\lambda^j}{j!} = e^{\lambda(e^t-1)}, \qquad (7.92)$$

the generating function is given by

$$\sum_{n=0}^{\infty} P_{n,\lambda}(x) \frac{t^n}{n!} \;\; = \;\; e^{xt} e^{-\lambda(e^t-1)}, \qquad (7.93)$$

where the polynomials also depend on λ. This leads to

$$e^{xt} e^{-\lambda(e^t-1)} \;\; = \;\; \sum_{n=0}^{\infty} \frac{t^n}{n!} e^{\lambda} \sum_{j=0}^{\infty} \frac{(j+x)^n(-\lambda)^j}{j!}.$$

Now the binomial theorem produces

$$e^{xt} e^{-\lambda(e^t-1)} \;\; = \;\; \sum_{n=0}^{\infty} \frac{t^n}{n!} \sum_{m=0}^{n} \binom{n}{m} x^{n-m} e^{-\lambda} \sum_{j=0}^{\infty} \frac{j^m(-\lambda)^j}{j!}.$$

Replacing j^m [1, entry 24.1.4B] by

$$j^m = \sum_{k=0}^{m} S(m,k)(j)_m = \sum_{k=0}^{m} S(m,k)j(j-1)\cdots(j-m+1),$$

where the $S(m,k)$ are *Stirling numbers* of the second kind [243], yields

$$e^{\lambda} \sum_{j=0}^{\infty} \frac{j^m(-\lambda)^j}{j!} \;\; = \;\; e^{\lambda} \sum_{k=0}^{m} S(m,k)(-\lambda)^m \sum_{j=m}^{\infty} \frac{(-\lambda)^{j-m}}{(j-m)!}$$

$$= \;\; \sum_{j=0}^{m} S(m,j)(-\lambda)^j.$$

The polynomial on the right-hand side is the mth *Bell polynomial* $B_m(-\lambda)$ [243]. Thus, we have a closed form for the Strodt polynomials:

$$P_{n,\lambda}(x) \;\; = \;\; \sum_{m=0}^{n} \binom{n}{m} \sum_{j=0}^{m} S(m,j)(-\lambda)^j \; x^{n-m}. \quad (7.94)$$

When $\lambda = -1$ and 1, the inner sum reduces to the mth *Bell number* and *complementary Bell number* [243], respectively. Again, we recover a corollary:

Proposition 7.82. *Let $P_{n,\lambda}(x)$ be defined by (7.94). Then*

$$e^{-\lambda} \sum_{j=0}^{\infty} P_{n,\lambda}(x+j) \frac{\lambda^j}{j!} \quad = \quad x^n \qquad (7.95)$$

and

$$\frac{d}{dx} P_{n,\lambda}(x) \quad = \quad n P_{n-1,\lambda}(x). \qquad (7.96)$$

(c) **Exponential distribution**. For $\lambda > 0$, we take the associated density function to be

$$g(u) \quad := \quad \left\{ \begin{array}{ll} \lambda e^{-\lambda u} & \text{for } u > 0 \\ 0 & u \leq 0 \end{array} \right. , \qquad (7.97)$$

and calculate the moment generating function

$$Q(t) \quad = \quad \lambda \int_0^{\infty} e^{ut - \lambda u} \, du = \frac{\lambda}{\lambda - t} \qquad (7.98)$$

for real $t < \lambda$. The generating function given by $\mathcal{S}_g(x^n)$, via Theorem 7.0, equals $e^{xt} \lambda / (\lambda - t)$. Therefore, by Theorem 7.0,

$$\sum_{n=0}^{\infty} \mathcal{S}_g(x^n) \frac{t^n}{n!} = \frac{e^{xt}}{1 - t/\lambda}. \qquad (7.99)$$

We thus have the following property of the images of x^n under the Strodt operator for the exponential distribution.

Proposition 7.83. *When $g(u)$ is the exponential density (7.97), the Strodt operator $\mathcal{S}_g$ applied to the monomial x^n gives a scaled Taylor series truncation of the exponential function:*

$$\mathcal{S}_g(x^n) = n! \lambda^{-n} \sum_{m=0}^{n} \frac{(\lambda x)^m}{m!}, \quad \text{for all } n \in \mathbb{N}_0, \lambda > 0. \quad (7.100)$$

Proof. On the right-hand side of (7.99), expand e^{xt} in a Taylor series and $(1 - t/\lambda)^{-1}$ in a geometric series. Then match t^n coefficients. $\qquad \square$

We claim that the Strodt polynomials for the exponential distribution are given by

$$P_{0,\lambda}(x) = 1, \quad P_{n,\lambda}(x) = x^n - nx^{n-1}/\lambda \quad \text{for } n \in \mathbb{N}. \quad (7.101)$$

Indeed,

$$\mathcal{S}_g\left(x^n - nx^{n-1}/\lambda\right) = \mathcal{S}_g(x^n) - n\mathcal{S}_g(x^{n-1})/\lambda \quad (7.102)$$

$$= n!\lambda^{-n} \sum_{m=0}^{n} \frac{(\lambda x)^m}{m!} - n!\lambda^{-n} \sum_{m=0}^{n-1} \frac{(\lambda x)^m}{m!} \quad (7.103)$$

$$= x^n \quad (7.104)$$

for $n \geq 1$, and $\mathcal{S}_g(1) = 1$. The justification for (7.102) is the linearity of the Strodt operator, and (7.103) follows from (7.100).

56. In each case in the development in Section 7.3.3, the proof relies on the fact that the function $V(s, h)$ can be related back to a polynomial from the original sequence. Is it possible to extend this process to a more general Strodt polynomials?

57. **Limits of Hermite polynomials**. Determine the asymptotic behavior of $H_n/H_n(1)$ where H_n denotes the n−th Hermite polynomial.

58. **Two iterations for π.** In a recent manuscript [158], Guillera produces a most concise accounting of the quartic algorithm for Pi given as [71, (3.1.8)] and of its quadratic counterpart. While the development is almost exactly what specialization of the general algorithms in [74, §5.5] yields, the reader is largely spared the need to digest the elliptic integral theory behind the general algorithm(s).

59. **Some test sums**. The goal is to succeed in evaluating the following sums with "generic" high-precision methods and as little special knowledge as possible.

   (a) Catalan constant:

$$G := \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2}.$$

   (b) Gregory constant:

$$\pi = 4 \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1}.$$

(c) Napier constant:

$$\log(2) \;=\; \sum_{n=0}^{\infty} \frac{(-1)^n}{n+1}.$$

and, putting all three together:

$$\sum_{n=1}^{\infty} (-1)^n \frac{\sum_{k=1}^{n} \frac{1}{k}}{2\,n+1} \;=\; G - \frac{1}{2}\,\pi\,\ln(2)\,.$$

(d) Euler constant:

$$\gamma \;=\; 1 + \sum_{k=2}^{\infty} \left\{ \frac{1}{k} + \ln\left(1 - \frac{1}{k}\right) \right\}.$$

(e) Slow sum:

$$\sum_{n=2}^{\infty} \frac{(-1)^n}{n\log(n)}.$$

(f) Abel sum:

$$\sum_{n=2}^{\infty} \frac{1}{n\log^2(n)}.$$

(g) Slow trigonometric series:

$$\sum_{n=1}^{\infty} \frac{\sin(nx)}{\sqrt{n}} \quad \text{and, for } 0 < x < \pi, \quad \sum_{n=1}^{\infty} \frac{\cos(nx)}{\sqrt{n}}.$$

(h) Hardy-Littlewood sum:

$$\sum_{n=1}^{\infty} \frac{\sin(x/n)}{n}.$$

(i) Euler sum:

$$\zeta(3) \;=\; \zeta(2,1) = 8\,\zeta(-2,1).$$

(j) Euler-Zagier sum [72, Chapter 3]:

$$\zeta(3,1,3,1) \;=\; \frac{2}{10!}\pi^8.$$

(k) Knuth sum:

$$\sum_{k=1}^{\infty}\left\{\frac{k^k}{k!e^k}-\frac{1}{\sqrt{2\pi k}}\right\} \;=\; -\frac{2}{3}-\frac{\zeta\left(\frac{1}{2}\right)}{\sqrt{2\pi}}.$$

(l) Madelung constant in two dimensions [72, Section 4.3.2.]:

$$4\,\zeta\left(\frac{1}{2}\right)\beta\left(\frac{1}{2}\right) \;=\; M_2 \;=\; \sum_{n=1}^{\infty}\frac{r_2(n)}{n^{1/2}},$$

where $\beta = L_{-4}$ is the Catalan zeta function. Moreover,

$$\beta\left(\frac{1}{2}\right) \;=\; \sum_{n=0}^{\infty}\frac{(-1)^n}{\sqrt{2n+1}}$$

and

$$\zeta\left(\frac{1}{2}\right) \;=\; (\sqrt{2}+1)\sum_{n=1}^{\infty}\frac{(-1)^n}{\sqrt{n}}.$$

(m) A slow e:

$$e-2 \;=\; \sum_{n=1}^{\infty}\frac{\left(n^2+2\,n\right)^{n+1}-n\,(n+1)^{2\,n+1}}{\left(n^2+n\right)^{n+1}}$$

(n) A subtle sinc sum:

$$\frac{1}{2}+\sum_{n=1}^{\infty}\prod_{k=0}^{7}\operatorname{sinc}\left(\frac{n}{2k+1}\right) \;=\; \int_0^{\infty}\prod_{k=0}^{7}\operatorname{sinc}\left(\frac{x}{2k+1}\right)\,dx.$$

60. **Normal (or not)?** In Section 4.3, we showed that the "hot-spot" lemma could be used to prove that the constant

$$\alpha \;=\; \alpha_{2,3} \;=\; \sum_{n=1}^{\infty}\frac{1}{3^n2^{3^n}}.$$

is 2-normal (see [39] for additional background and details). One question that can be raised here is whether this constant is b-normal (or not) for other bases b.

To that end, it is illuminating to explicitly calculate the first few hundred base-b digits of α for various bases b. This can be done

easily in *Mathematica* or *Maple*, or by using one's own computer code coupled with high-precision arithmetic software such as the ARPREC software available at `http://www.experimentalmath.info`. When this is done, it is clear that the base-b digits of this constant are *not* random for certain bases, beginning, for instance, with base 6.

This question can be explored analytically as follows. Let the notation $\{\cdot\}$ denote fractional part. Note that the base-6 digits immediately following position n in the base-6 expansion of α can be obtained by computing $\{6^n \alpha\}$, which can be written as follows:

$$\{6^n \alpha\} = \left\{ \sum_{m=1}^{\lfloor \log_3 n \rfloor} 3^{n-m} 2^{n-3^m} \right\} + \left\{ \sum_{m=\lfloor \log_3 n \rfloor+1}^{\infty} 3^{n-m} 2^{n-3^m} \right\}.$$

Now note that the first portion of this expression is *zero*, since all terms of the summation are integers. In the case when $n = 3^M$, where $M \geq 1$ is an integer, we see that the first term of the second expression is

$$3^{3^M-(M+1)} 2^{3^M-3^{M+1}} = 3^{3^M-M-1} 2^{-2\cdot 3^M} = \frac{\left(\frac{3}{4}\right)^{3^M}}{3^{M+1}}.$$

We can bound the sum of all terms of the second summation by $(1+\epsilon)$ times this amount, for all sufficiently large M. Thus, we can write

$$\{6^{3^m} \alpha\} \approx \frac{\left(\frac{3}{4}\right)^{3^m}}{3^{m+1}},$$

and this approximation is as accurate as one wishes (in ratio) for all sufficiently large m.

Given the very small size of the expression $(3/4)^{3^m}/3^{m+1}$ for even moderate-sized m, it is clear the base-6 expansion will have very long stretches of zeroes beginning at positions $3^m + 1$. This reckoning can be made rigorous by noting that for any $\epsilon > 0$, there is some M such that for all $m > M$ we have

$$3^m \left[\log_6 \left(\frac{3}{4}\right) - \epsilon \right] < Z_m < 3^m \left[\log_6 \left(\frac{3}{4}\right) + \epsilon \right]$$

where Z_m is the length of this segment of zeroes beginning at position $3^m + 1$. By estimating the sum of Z_m up to some M, one can conclude that the fraction of zeroes in the first n base-6 digits of $\alpha_{2,3}$ must, infinitely often, exceed

$$\frac{4}{3} \cdot \frac{\log_6 \left(\frac{3}{4}\right)}{1 + \log_6 \left(\frac{3}{4}\right)} \approx 0.18446111\ldots,$$

which is clearly greater than $1/6$. This means that α is not 6-normal. Complete details are given by Bailey [21].

Can you identify other bases b for which α is not b-normal?

61. For $n = 1, 2, \cdots, 30$, in each case, recover the minimal polynomial of $\alpha_n := (2^n + 1)^{1/n}$ from a sufficiently precise numerical value for α_n. Then perform the same task for $\beta_n := (2^{1/n} + 1)^n$. Compute the Euclidean norm of the consequent polynomials and observe that for β_n this gives a very misleading indicator of the complexity of the number.

62. **More on Bessel moments**. Larry Glasser has observed that

$$c_{4,0} \quad = \quad \int_0^\infty K_0^4(t)\, dt = \pi \int_0^1 \frac{K^2(k)}{k'}\, dk$$

(a) Hence, derive that

$$c_{4,0} \quad = \quad \pi \int_0^{\pi/2} K^2\left(\cos(t)\right) dt \quad = \quad \frac{\pi^4}{4}\, {}_4F_3\left(\begin{array}{c} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{array}\bigg| 1\right)$$

$$= \quad \frac{\pi^4}{4} \sum_{n=0}^\infty \frac{\binom{2n}{n}^4}{4^{4n}}.$$

(b) Conjecture that $c_{4,2m}$ can be expressed as

$$c_{4,2m} \quad \overset{?}{=} \quad \frac{\pi^4}{4} \sum_{n=0}^\infty p_m\left(\frac{1}{n+1}\right) \frac{\binom{2n}{n}^4}{4^{4n}},$$

for polynomials of some fixed degree. Explore the sequence p_m by using PSLQ and the recursion

$$4(5k^3 + 3k)\, c_{4,k+2} - (k-1)^5\, c_{4,k} \quad = \quad 64(k+1)c_{4,k+2}$$

of Section 7.2.3.

(c) A corresponding derivation gives

$$c_{3,0} \quad = \quad \int_0^\infty K_0^3(t)\, dt = \pi \int_0^1 \frac{K(k)}{k'\sqrt{1+3k^2}}\, dk.$$

Hence confirm—or indeed deduce—that

$$c_{3,0} \quad = \quad \frac{\sqrt{3}\pi^3}{8}\, {}_3F_2\left(\begin{array}{c} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{array}\bigg| \frac{1}{4}\right) = \frac{\sqrt{3}\pi}{2} K^2(k_3)$$

where $k_3 = \sin(\pi/12)$ is the third singular value (see [25, pp. 238–247] for details).

Hint: the required identity reduces to

$$\sum_{n=0}^{\infty} \frac{\binom{2n}{n}^3}{4^{3n}} \, {}_2F_1\left(\begin{array}{c} \frac{1}{2}, \frac{1}{2} \\ n+1 \end{array} \middle| \frac{3}{4} \right) = \sqrt{3} \, {}_3F_2\left(\begin{array}{c} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{array} \middle| \frac{1}{4} \right).$$

One can also establish that

$$c_{3,2} = \frac{1}{9} c_{3,0} - \frac{\pi^4}{24} c_{3,0}^{-1},$$

and so via the recursion of Section 7.2.3 obtain all even $c_{3,2m}$.

(d) For completeness, we record [74]

$$\int_0^1 \frac{K(k)}{k'} \, dk = K^2\left(\frac{1}{\sqrt{2}} \right).$$

(e) Broadhurst has shown that

$$c_{5,1} = \int_0^{\frac{1}{3}} 4x \, K(y)$$

$$\times \frac{\left(\frac{\pi^2}{12} - \mathrm{Li}_2\left(\frac{1}{2} - \frac{\sqrt{1-4x^2}}{2} \right) + \frac{1}{2} \ln^2\left(\frac{1}{2} - \frac{\sqrt{1-4x^2}}{2} \right) - \ln^2(x) \right)}{\sqrt{(1+3x)(1-x)^3(1-4x^2)}} \, dx,$$

where $y := \sqrt{\frac{(1-3x)(1+x)^3}{(1+3x)(1-x)^3}}$. Can this representation be further reduced? There is a corresponding more complicated integral for $c_{5,3}$ and $c_{5,5}$.

(f) The corresponding closed form, for a so-called sunrise integral (see also Exercise 12), is known empirically thanks to the remarkable insight of David Broadhurs [92]:

$$\int_0^{\infty} x \, I_0(x) \, K_0^4(x) \, dx = \frac{\pi}{2\sqrt{15}}$$

$$\times K\left(\frac{\sqrt{2}}{16} \left(2 - \sqrt{3} \right) \left(\sqrt{5} + \sqrt{3} \right) \left(3 + \sqrt{5} \right) \right)$$

$$\times K\left(\frac{\sqrt{2}}{16} \left(2 - \sqrt{3} \right) \left(\sqrt{5} - \sqrt{3} \right) \left(3 - \sqrt{5} \right) \right).$$

63. Prove for $|z| < 1/\sqrt{2}$, as suggested by Larry Glasser [146], that

$$\frac{z \arcsin(z)}{(1 - 2z^2)\sqrt{1 - z^2}} = \sum_{n=1}^{\infty} \left(\sum_{k=1}^{n} \frac{2^{k+n-1}}{k\binom{2k}{k}} \right) z^{2n}.$$

64. **The p-adic Gamma function** [283, Section 6.2]. The function Γ_p is defined for a prime p as the unique continuous extension to Z_p of

$$\Gamma_p(n) \quad := \quad (-1)^n \prod_{k=1,\, p \nmid k}^{n} k,$$

defined on N.

(a) For odd n, we have

$$(-1)^{(n-1)/2} \prod_{k=1}^{n} \Gamma_p\left(\frac{k}{n}\right) = \left(\frac{p}{n}\right) \qquad (7.105)$$

if p does not divide n, as discovered experimentally and proven by Villegas [283, Proposition 6.3]. For n even, there is a corresponding formula, but it adds a factor $\Gamma_p(1/2)^{n-1}$ on the right.

(b) However, even though

$$\Gamma_p\left(\frac{1}{2}\right)^2 = -\left(\frac{-4}{p}\right)$$

for all odd primes, the sign of $\Gamma_p(1/2)$ appears very random. Using code for Γ_p (see [283, Section 6.2]) along with code such as

```
with(numtheory)::L:=[seq(-jacobi(-4,ithprime(n)),
  n=2..100)];
```

in *Maple*, can one find any structure therein?

65. **Two harmonic sums.** Identify and prove the values of $\sum_{n>0} 2^{-n} H_n/n$ and $\sum_{n>0} [1 + 2(-1)^n] H_n/n^4$, where $H_n = 1 + 1/2 + \cdots + 1/n$ is the sum of the harmonic numbers.
    Hint: both are combinations of ζ-function values.

66. **Some cautions from Villegas.** In Exercise 38 and elsewhere in [25, 71, 72] we have shown some cautionary examples regarding "the law of small numbers." Here are some fine additions [283]:

(a) Euler's *Exemplum Memorabile Inductionis Fallacis* [283, p. 121]. Define *trinomial numbers* as $t_n := [x^0](x + 1 + 1/x)^n$, where the $[x^j]$ notation denotes the coefficient of that power. Find a closed form, the generating function, and a three-term recursion for $\{t_n\}$. Generate sufficient trinomial numbers to identify the sequence in Sloane. Confirm Euler's observation that for $n = 0, 1, \ldots, 8$ that $3t_{n+1} - t_{n+2} = F_n(F_n + 1)$, where F_n is the nth Fibonacci number, but fails subsequently.

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

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

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

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

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

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

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

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

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

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

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

$$[1], \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix}, \begin{bmatrix} 1 & 2 & 3 \\ 2 & 5 & 9 \\ 3 & 9 & 19 \end{bmatrix}, \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 9 & 14 \\ 3 & 9 & 19 & 34 \\ 4 & 14 & 34 & 69 \end{bmatrix}, \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 5 & 9 & 14 & 20 \\ 3 & 9 & 19 & 34 & 55 \\ 4 & 14 & 34 & 69 & 125 \\ 5 & 20 & 55 & 125 & 251 \end{bmatrix}.$$
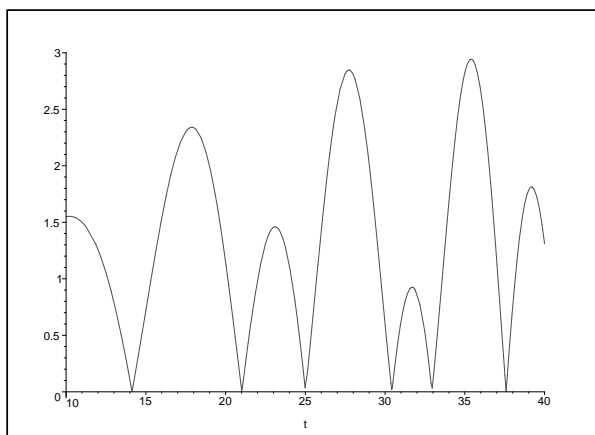
Figure 7.16. The first few zeros of ζ on the critical line.

68. **The Riemann hypothesis as a random walk** [80]. Recall the
    Liouville lambda function $(\lambda(s) := \sum_{n>0}(-1)^{r(n)}/n^{-s}$, where $r(n)$
    counts the number of prime factors in n). Figure 68 shows λ plotted
    as a two-dimensional "random walk," by walking $(\pm 1, \pm 1)$ through
    pairs of points of the sequence, $\{\lambda(2k), \lambda(2k+1)\}_{k=1}^n$. The fact that n
    steps of the walk stay in a box with side of length roughly $\sqrt{n}$ implies
    the *Riemann hypothesis*: that all nonreal zeros of the ζ-function have
    a real part equal to one half (the *critical line*). The first few are
    plotted in Figure 67. See Figure 2.20 for another graphical equivalent.
    Show (see, for example [74, p. 300]) that

    $$\sum_{n=1}^{\infty} \frac{\lambda(n)}{n^s} = \frac{\zeta(2s)}{\zeta(s)}.$$

69. **Gordon's identity**. Confirm Gordon's identity

    $$\frac{\sum_{m=-\infty}^{\infty} (6\,m+1)\,q^{(6\,m+1)^2}}{\sum_{m=-\infty}^{\infty} (-1)^m\,q^{(6\,m+1)^2}} = \theta_4^2(q^{24}) \qquad (7.106)$$

    and so derive a recursion for $r_2(n)$ (see [74, Section 9.4]). Find prod-
    uct forms for all three series in the identity (7.106).

70. **A partial fraction due to Euler**. Discover and prove the closed
    form of the partial fraction decomposition for $x^{-s}(1+x)^{-t}$ with non-
    negative integers $s \geq 0, t \geq 0, s + t \geq 1$ (see [72, Lemma 3.6]).
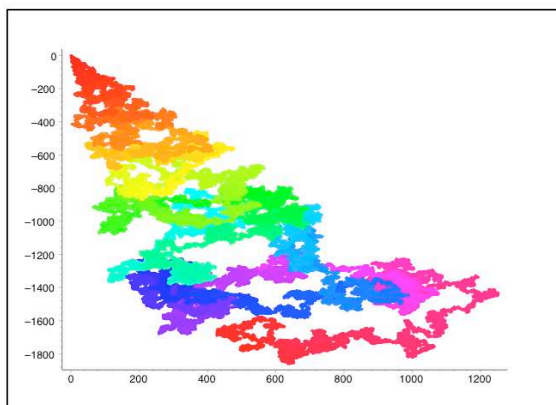
Figure 7.17. Riemann Hypothesis as a random walk on Liouville's function.

71. **The logistic curve**. We briefly discussed the bifurcations of the logistic curve [129] in Section 2.3 and in [25, Section 8.3]. For the limiting case, this yields the dynamical system

$$x_{n+1} := 4x_n(1 - x_n) \qquad (7.107)$$

on the interval $[0, 1]$.

(a) Show that a closed form for $f^{(n)}(x)$ with initial value x is

$$x \mapsto \frac{1}{2}\left\{1 - \cos(2^n \arccos(1 - 2x))\right\}.$$

Indeed, the specific map in (7.107) is one of the easiest to show *chaotic* (see [129] and [25, p. 288]). The core task is to determine that the *Lyapunov exponent*, which in good cases given by $\lambda_f(x) := \lim_{n\to\infty} \frac{df^{(n)}(x)}{dx}$, is strictly positive except countably as orbits then disperse.
Hint: consider the substitution $\sin(\theta_n) = x_n$ and note that a chain rule argument shows the exponent is usually unchanged by smooth *conjugacy*: $g = \phi^{(-1)} f \phi$.

(b) Empirically determine the value(s) of $\lambda_f(1)$.
Hint: $1/2 - 1/(2\sqrt{2})$ iterates to $1/2$ and then to 1. The Lyapunov exponent appears to be $2\log 2$.

(c) Deduce that

$$\lim_{n\to\infty} \frac{\log|\sin(2^n)|}{n} = 0$$
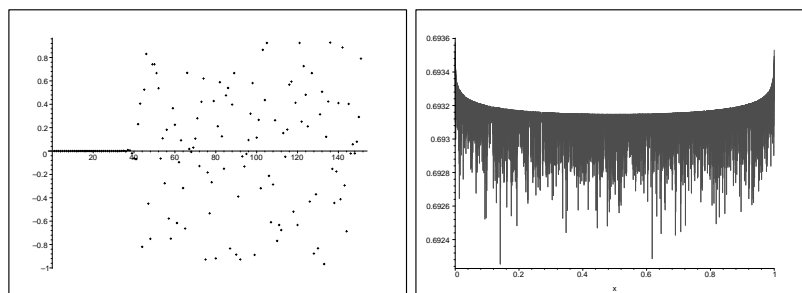
Figure 7.18. Scatter from 150 iterates of $x_0 + .1^{14}$ and $x_0 := (1 - \cos 1)/2$, and Lyapunov exponent plotted from 10^4 iterations.

if and only if $\lambda_f\left((1 - \cos 1)/2\right) = \log 2$. Thus, as observed by Stan Wagon, we connect a nontrivial number theory result to information about the bit string of $1/\pi$, without needing an irrationality estimate for π [74].

Hint: for $x = (1 - \cos 1)/2$ we conjugate to $1/\pi$. See also Figure 71.

72. **Irrationality estimates** can apparently not prove the prior result easily. The best one can obtain directly appears to be an order estimate:

Proposition 7.84. *For each $\delta > 0$,*

$$\lim_{n \to \infty} \frac{\log(|\sin 2^n|)}{n^{1+\delta}} = 0,$$

while for $\delta = 0$, the $\limsup$ and $\liminf$ of the expression lie between $-9 \log 2$ and 0. For $\delta < 0$, the limit is ∞.

Proof. Given any positive integer n, choose an integer q such that $|q\pi - 2^n| < \pi/2$. Then, by Hatta's improvement [74, Section 11.2] of Mahler's theorem,

$$|\sin 2^n| = \sin(|q\pi - 2^n|) > \frac{2}{\pi}(|q\pi - 2^n|) > \frac{2}{\pi q^9}.$$

Hence $0 > \log(|\sin 2^n|) > \log(2/\pi) - 9\log q > \log(2/\pi) - 9\log \frac{2^n + \pi/2}{\pi}$. Since

$$\lim_{n \to \infty} \frac{1}{n} \log \frac{2^n + \frac{\pi}{2}}{\pi} = \log 2,$$

the proposition follows.

73. **Spin integrals: theory**. Correlation integrals for a spin-1/2 anti-ferromagnet have received much recent attention. As given by Boos and Korepin, for a length-n spin chain, we consider [58, equation 2.2]

$$P(n) \quad := \quad \frac{1}{(2\pi i)^n} \int_{\mathcal{C}^n} U_n T_n \; \mathcal{D}\vec{\lambda}, \tag{7.108}$$

where

$$U_n \quad := \quad \pi^{n(n+1)/2} \frac{\prod_{j<k} \sinh \pi(\lambda_k - \lambda_j)}{\prod_j \sinh^n \pi \lambda_j} \tag{7.109}$$

and

$$T_n \quad := \quad \frac{\prod_j \lambda_j^{j-1} (\lambda_j + i)^{n-j}}{\prod_{j<k} (\lambda_k - \lambda_j - i)}. \tag{7.110}$$

The nomenclature is as follows. Lone indices such as j run over $[1, n]$. The constraint $j < k$ means $1 \le j < k \le n$. The "curly-D" notation is simply, for an arbitrary vector r, $\mathcal{D}\vec{r} := dr_1 \cdots dr_n$. The integration domain $\mathcal{C}^n$ denotes that each λ_j runs eastward along the horizontal contour $\mathcal{C} := \{x - i/2 : x \in (-\infty, \infty)\}$.

The general closed form for $P(n)$ is still open. Currently, all $P(n)$ for $n \le 6$ have been found [59, 60, 58, 189, 61]. Each such evaluation involves rational-weighted sums of products of odd-argument η (or *alternating* ζ) functions, where

$$\eta(s) \quad := \quad \left(1 - 2^{1-s}\right) \zeta(s),$$

with ζ denoting the Riemann zeta function. Note that $\eta(-1) = 1/4$, $\eta(1) = \log 2$. It is known, for example, that

$$P(3) \quad = \quad \eta(-1) - \eta(1) + \frac{1}{2}\eta(3) = \frac{1}{4} - \log 2 + \frac{3}{8}\zeta(3),$$

while the most advanced known case as of this writing is [61, equation 4.3]

$$P(6) \quad = \sum_{\substack{a \le b \le c \\ a,b,c \, \in \, (-1,1,3,5,7,9)}} q_{a,b,c} \; \eta(a) \; \eta(b) \; \eta(c),$$

where the $q_{a,b,c}$ are all rational.[2] Note that we are exploiting the fact of $\eta(-1)$ being rational to effect an η-sum that is perhaps more symmetrical than those in the literature. Indeed, the rational leading term here for $P(6)$ is $q_{-1,-1,-1}\eta(-1)^3$.

The original *Boos–Korepin conjecture* [59] states that $P(n)$ is always a combination of η evaluations as above. This conjecture has since been interpreted in a "strong" form, postulating the algebraic character of the η combinations entering into $P(n)$ [61, equations 4.5, 4.6] and is settled by Boos and colleagues in [57]. However, that resolution can be considered nonconstructive: there is still no effective form for the general coefficients, and certain asymptotic properties of $P(n)$ remain elusive. For example, it is suggested in [60] that

$$P(n) \quad \sim \quad a^{-n^2},$$

with a estimated from what are known as DMRG computations as $a \approx 1.6719 \pm 0.0005$. Using *quasi-Monte Carlo* (qMC) methods as in [22] on the relatively stable integrands given in Exercise 74, $a \approx 1.67$ has been verified. Computation of the integrals to extreme precision (100 or more digits) can resolve the values of the rational coefficients via integer relation detection algorithms such as PSLQ.

74. **Spin integrals: numerics**. One difficulty for the numerical quadrature of (7.108) is the complex character of the variables; another is the infinite domain of integration. The substitutions

$$\lambda_j \quad = \quad x_j - i/2, \quad x_j = \frac{1}{\pi}a_j, \quad a_j =: \frac{1}{2}\log\frac{1+v_j}{1-v_j}$$

handle both and yield an integral over vectors $\vec{v}$ in the cube $[-1,1]^n$:

$$P(n) \quad = \quad \frac{(-1)^{\lfloor\frac{n}{2}\rfloor}}{(2\pi)^n}\int_{[-1,1]^n}\mathcal{D}\vec{v}\prod_j\left(1-v_j^2\right)^{n/2-1}\left(a_j - \frac{i\pi}{2}\right)^{j-1}$$

$$\times\left(a_j + \frac{i\pi}{2}\right)^{n-j}\prod_{1\leq k<h\leq n}\frac{\sinh(a_h-a_k)}{a_h-a_k-i\pi}. \qquad (7.111)$$

The natural quadrature setup, then, is to assume each variable v_j of integration will lie in $(-1,1)$, and when evaluating the integrand, to create the a_j from the v_j via the logarithmic formula above. Note

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[2]And yet, as one of the many open mysteries in regard to the $P(n)$, the coefficients $q_{1,5,7}$ and $q_{1,3,3}$ vanish in the $P(6)$ evaluation, whereas $q_{3,3,3}$, historically expected to vanish, does not [61].

that if $\vec{v}$ is on any face of the cube—i.e., some $v_j = \pm 1$, the logarithm is singular, but one may take the integrand to be 0 at such points. Note that $P(n)$ is always *real*—from symmetry arguments—so one may either use complex arithmetic for the integrand and keep only the real part, or prereduce this integrand symbolically. There are various speedups for the integral (7.111), such as table lookup for pairs $(k, h > k)$ and some reductions, such as

$$\sinh(a_h - a_k) = \frac{v_h - v_k}{\sqrt{1 - v_h^2}\sqrt{1 - v_k^2}},$$

which avoids some of the transcendental arithmetic. Indeed, the square root terms largely cancel, leaving us with

$$P(n) = \frac{(-1)^{\lfloor \frac{n}{2} \rfloor}}{(2\pi)^n} \int_{-1,1]^n} \mathcal{D}\vec{v} \prod_j \left(1 - v_j^2\right)^{-1/2} \left(a_j - \frac{i\pi}{2}\right)^{j-1}$$

$$\times \left(a_j + \frac{i\pi}{2}\right)^{n-j} \prod_{1 \le k < h \le n} \frac{v_h - v_k}{a_h - a_k - i\pi}. \qquad (7.112)$$

If one desires some singularity removal for reasons of numerical stability, the substitutions $v_j := \sin \phi_j$ yield

$$P(n) = \frac{(-1)^{\lfloor \frac{n}{2} \rfloor}}{(2\pi)^n} \int_{-\pi/2}^{\pi/2} \cdots \int_{-\pi/2}^{\pi/2} \mathcal{D}\vec{\phi} \qquad (7.113)$$

$$\times \prod_j \left(a_j - \frac{i\pi}{2}\right)^{j-1} \left(a_j + \frac{i\pi}{2}\right)^{n-j} \prod_{1 \le k < h \le n} \frac{\sin \phi_h - \sin \phi_k}{a_h - a_k - i\pi},$$

where now

$$a_j = \frac{1}{2} \log \frac{1 + \sin \phi_j}{1 - \sin \phi_j}.$$

The formulation (7.113) is well suited for high-precision quadrature: it is free from singularities (provided one stays away from certain rational values with removable singularities), and is defined on a finite multidimensional cube. Since the integrand is *regular* (free from singularities and vertical derivatives), we found ordinary multidimensional Gaussian quadrature is the best quadrature scheme to use. However, run time very rapidly increases with increasing dimension, due to the need for roughly N^m evaluations of the integrand function, where N is the number of one-dimensional evaluations and m is the dimension.

In order to keep calculations to a minimum, we employed a number of techniques. It was particularly helpful to precompute each part of the expression in (7.113), including the $(a_j - i\pi/2)^{j-1}$ terms, the sin terms and even the denominator of the right-most term (stored as a two-dimensional array). We also employed a binary search technique to quickly retrieve the requisite value from our tables. Even with these changes, these computations are extremely expensive. We were able to compute $P(n)$ to at least modest precision for n up to 6; beyond this level seems impractical using our current methods. The run times and processors used shown in the Table 74 underscore the rapidly escalating difficulty of these computations.

n	Digits	Processors	Run Time
2	120	1	10 sec
3	120	8	55 min
4	60	64	27 min
5	30	256	39 min
6	6	256	59 hrs

Table 7.1. Run times for computing multidimensional spin integrals.

75. **An AGM binary operation** [273]. Define a binary operation on the positive real numbers as follows: for $a, b > 0$ there is a unique q in $(-1, 1)$ such that $M(a, b) = 1/\theta_3^2(q)$, where $M(a, b)$ is the *arithmetic-geometric mean* limit of Gauss discussed in Section 5.6.2 as well as by Borwein and Borwein [74, Section 2.1]. Define $*$ by $a*b = \theta_4^2(q)/\theta_3^2(q)$. Show that

(a) $1 * a = a$ ($*$ is unital); $a * a = b * b$ implies $a = b$ and $a * b = M(a, b) * M(a * b) = b * a$ (commutation).

(b) $a * c = a * c$ implies $b = c$ (cancellation); $(a * b) * (a * c) = a * (a(b * c))$ (distribution).

(c) If $c := a * b$ then $c = b\left(b^{-1} * (b^{-1}a)\right)$. Therefore, the $*$-inverse of a is $a\left(a^{-1} * a^{-1}\right)$.

(d) Show that $*$ is not associative.

(e) Show that $(2n + 1) * (2 * n^2 + 2 * n + 1) = (2 * n + 1)^2$ is not associative.

(f) Define $*$ in terms of elliptic integrals.

76. **An open question about the Lambert function** [114]. The function $u(w)$ that solves

$$w^2 = -2u - 2\log(1-u)$$

and has $u(0) = 0$ is analytic at 0 and of independent interest because it arises in one approach to large-scale computation of zeros of Riemann's ζ. First, note the function

$$f(u) := \frac{-2u - 2\log(1-u)}{u^2} - 1 = \sum_{n=1}^{\infty} \frac{2u^n}{n+2}$$

is analytic at the origin, while $f(0) = 0$, and

$$|f(u)| < f\left(\frac{1}{2}\right) < 1 \text{ for } |u| < \frac{1}{2}.$$

Hence, $w(u) := u\big(1 + f(u)\big)^{1/2}$ is analytic at $u = 0$, since $z \mapsto (1 + z)^{1/2}$ is analytic at $z = 0$. The discussion by Ahlfors on[3, p. 75] along with his Corollary 2 [3, p. 132], implies that $g(w) = u^{-1}(w)$ is analytic at zero because w is analytic while $w'(0) = 1$. Indeed a continuous selection is $\text{LambertW}\left(-e^{-1/2\,w^2-1}\right)+1$. Thus, the series for $u(w)$ converges in some complex neighborhood of zero and so has a positive radius of convergence. Moreover, the series of u begins

$$w - \frac{1}{3}w^2 + \frac{1}{36}w^3 + \frac{1}{270}w^4 + O\left(w^5\right),$$

and the coefficients are generated by $a_1 := 1$ and

$$(j+1)a_j = -a_{j-1} + \sum_{k=2}^{j-1} k\, a_k a_{j-k+1}.$$

Experiments suggest ρ, the radius of convergence is in $[3, 4]$. The discussion by Corless, Jeffrey, and Knuth [114, Section 3.1] mistakenly asserts that the radius is infinite. A recent conjecture of those authors is $\rho = 2\sqrt{\pi} = 3.544907702\ldots$. This is consistent with our numerical estimate of 3.531. Can one corroborate this to reasonable precision or, ideally, prove it is correct with an effective estimate of the error?

77. **The proof of a longstanding MZV conjecture** [294]. In 1996, Borwein and Broadhurst discovered, using PSLQ, the conjectured identity

$$8^N \zeta\left(\{-2,1\}_N\right) \overset{?}{=} \zeta\left(\{2,1\}_N\right). \tag{7.114}$$

for $N = 1, 2, 3, \cdots$. The notation should be clear: curly brackets denote repetition and negative denote entries alternating signs. Such alternating sums are called *multivariate zeta values* (MZVs), while sums with all-positive terms are named *Euler sums*, after Euler who first studied them in detail. The first two cases are

$$8 \sum_{n>m>0} \frac{(-1)^n}{n^2 m} = \sum_{n>m>0} \frac{1}{n^2 m} = \sum_{n>0} \frac{1}{n^3}$$

and

$$64 \sum_{n>m>o>p>0} \frac{(-1)^n (-1)^o}{n^2 m \, o^2 p} = \sum_{n>m>o>p>0} \frac{1}{n^2 m o^2 p} = \sum_{n>m>0} \frac{1}{n^3 m^3}.$$

The problem lies in the left-hand identities. We discussed this conjecture in detail in *Experimental Mathematics in Action* [25, Example 1.5], where we showed that, proof or no proof, the experimental evidence in favor of this conjecture is overwhelming.

In this guided exercise, graciously provided by David Bradley, we outline a subtle recent proof by Zhao [294]. Set

$$a = \frac{dt}{t}, \qquad b = \frac{dt}{1-t}, \qquad c = \frac{-dt}{1+t}.$$

For every positive integer n, define

$$\beta_n = a^{n-1} b \quad \text{and} \quad \gamma_n = a^{n-1} c.$$

Set $A_0 = \{\mathbf{1}\}$ to be the set of empty word. Define $\mathfrak{A} = \mathbf{Q}\langle \mathbf{A} \rangle$ to be the graded noncommutative polynomial $\mathbf{Q}$-algebra generated by the letters a, b, and c, where A is a locally finite set of generators whose degree n part A_n consists of words (i.e., a monomial in the letters) of length n. Let $\mathfrak{A}^0$ be the subalgebra of $\mathfrak{A}$ generated by words not beginning with b and not ending with a. The words in $\mathfrak{A}^0$ are called *admissible words*. Every Euler sum is expressible as an iterated integral over $[0, 1]$ of a unique admissible word w in $\mathfrak{A}^0$, denoted $Z(w)$.

(a) Show that

$$\zeta(s_1, \ldots, s_l) \quad = \quad Z(\beta_{s_1} \cdots \beta_{s_l}).$$

For example, show that

$$\zeta(\{3\}^n) \quad = \quad Z\big((a^2 b)^n\big).$$

(b) If some s_i are replaced by $\bar{s}_i$ in part (a), then we need to change some β's to γ's. Find the rule of this correspondence. Then use this rule to verify that for any positive integer n,

$$\zeta(\{\bar{2},1\}^n) \quad = \quad (ac^2ab^2)^{[n/2]}(ac^2)^{2\{n/2\}}.$$

Here, for a positive real number x, $[x]$ and $\{x\}$ are the integral part and the fractional part of x, respectively.

(c) (A *distribution relation*.) Show that

$$Z\big((a^2(b+c))^n\big) \quad = \quad \frac{1}{4^n}\zeta(\{3\}^n).$$

Denote by $\mathfrak{A}^1$ the subalgebra of $\mathfrak{A}$ generated by words β_k and γ_k with $k \geq 1$. In other words, $\mathfrak{A}^1$ is the subalgebra of $\mathfrak{A}$ generated by words not ending with a. For any word $w \in \mathfrak{A}^1$ and positive integer n, define the toggling operator $\tau_{\beta_n}(w) = w$, and $\tau_{\gamma_n}(w)$ to be the word with β and γ toggled. For example $\tau_{\gamma_1}(\gamma_2\beta_4) = \beta_2\gamma_4$. We then define a new multiplication $*$ on $\mathfrak{A}^1$ by requiring that $*$ distribute over addition, that $1*w = w*1 = w$ for any word w; and that, for any words w_1, w_2 and special words x and y equaling either β_n or γ_m (for some n, m),

$$xw_1 * yw_2 \quad = \quad x\Big(\tau_x\big(\tau_x(w_1) * yw_2\big)\Big) + y\Big(\tau_y\big(xw_1 * \tau_y(w_2)\big)\Big)$$
$$+ \quad [x,y]\Big(\tau_{[x,y]}\big(\tau_x(w_1) * \tau_y(w_2)\big)\Big),$$

where

$$[\beta_m, \beta_n] = [\gamma_m, \gamma_n] = \beta_{m+n}, \quad \text{and} \quad [\gamma_m, \beta_n] = [\beta_m, \gamma_n] = \gamma_{m+n}.$$

We call this multiplication the *stuffle product*.

(d) Show that for any two words $w_1, w_2 \in \mathfrak{A}^0$,

$$Z(w_1)Z(w_2) \quad = \quad Z(w_1 * w_2).$$

For any letters x and y and words w, w_1, and w_2, define recursively: $w \text{ш} 1 = 1 \text{ш} w = w$ and

$$(xw_1)\text{ш}(yw_2) \quad = \quad x\Big(w_1\text{ш}(yw_2)\Big) + y\Big((xw_1)\text{ш}w_2\Big).$$

(e) Show that for any two words $w_1, w_2 \in \mathfrak{A}^0$,

$$Z(w_1)Z(w_2) \quad = \quad Z(w_1\text{ш}w_2).$$

For any two words $w_1, w_2 \in \mathfrak{A}^1$, set

$$\text{ш}[w_1, w_2] \quad = \quad w_1 \text{ш} w_2, \quad \text{and} \quad *[w_1, w_2] = w_1 * w_2.$$

For any positive integer i, define the ith cut of a word $l_1 \ldots l_m$ (where l_i are letters) to be a pair of words given by

$$\text{Cut}_i[l_1 l_2, \ldots l_m] = \begin{cases} \big[(l_1, l_2, \ldots, l_i), (l_{i+1}, \ldots, l_m)\big] & \text{if } i \text{ is odd,} \\ \big[(l_i, \ldots, l_2, l_1), (l_{i+1}, \ldots, l_m)\big] & \text{if } i \text{ is even,} \end{cases}$$

for $i = 0, \cdots, m$. Here by convention for empty word $\mathbf{1}$, we have $[w, \mathbf{1}] = [\mathbf{1}, w] = w$. Then we can define the composites $\text{ш}_i = \text{ш} \circ \text{Cut}_i$, $*_i = * \circ \text{Cut}_i$, and the difference $\Delta_i = \text{ш}_i - *_i$. For any two words l_1 and l_2, define the $\star$-concatenation by setting $l_1 \star l_2 = l_1 l_2$ except that

$$b \star b = bc, \quad \text{and} \quad c \star c = cb.$$

(f) Prove by induction that for every positive integer n,

$$\sum_{i=0}^{2n} (-1)^i *_i \big((cd)^{\star n}\big) \quad = \quad (-1)^n (a^2(b+c))^n.$$

Here $d = a(b+c)$ is regarded as one letter when we do the cuts first, retaining the $\star$-concatenation. Note that $d \star b = d \star c = a(cb + bc)$.

(g) Prove by induction that for every positive integer n,

$$\sum_{i=0}^{2n} (-1)^i \text{ш}_i \big((cd)^{\star n}\big) \quad = \quad (-2)^n (ac^2 ab^2)^{[n/2]} (ac^2)^{2\{n/2\}}$$

and

$$\sum_{i=0}^{2n} (-1)^i \text{ш}_i \big((bd)^{\star n}\big) \quad = \quad (-2)^n (ab^2 ac^2)^{[n/2]} (ab^2)^{2\{n/2\}}.$$

(h) Finally, prove that for every positive integer n,

$$\zeta(\{3\}^n) \quad = \quad 8^n \zeta(\{\overline{2}, 1\}^n).$$

78. **Continued fractions with n limit points**. When a continued fraction diverges, it may diverge with surprising structure and regularity, as in the case of the *Stern-Stolz* Theorem [177], which states that if

$\{b_n\}$ is a sequence of numbers whose sum converges absolutely, then the convergents P_n/Q_n of the continued fraction

$$b_0 + \frac{1}{b_1} + \frac{1}{b_2} + \frac{1}{b_3} + \cdots$$

converge to two different limits, depending on the parity of n. More precisely, there are constants A_0, A_1, B_0, B_1 with $A_1 B_0 - A_0 B_1 = 1$ such that for $k \in \{0, 1\}$,

$$\lim_{n\to\infty} P_{2n+k} = A_k, \qquad \lim_{n\to\infty} Q_{2n+k} = B_k.$$

(a) The Stern-Stolz Theorem does not apply to the continued fraction

$$F := \frac{-1}{1+q} + \frac{-1}{1+q^2} + \frac{-1}{1+q^3} + \cdots,$$

with $|q| < 1$, given in compact form and found in Ramanujan's Lost Notebook [239, p. 45]. Ramanujan gave a closed form for the limit points of F, which was first proven by Andrews, Berndt, Sohn, Yee, and Zaharescu [7]. Explore the convergence properties of F. Is it possible to experimentally recover Ramanujan's evaluation? What happens when q is replaced by $1/q$?

(b) Bowman and McLaughlin [84] generalized Ramanujan's continued fraction and used infinite products of matrices to construct a class of continued fractions with n limit points, for arbitrary n. A special case of their theorem is the fraction

$$\frac{-ab}{a+b+p_1} + \frac{-ab}{a+b+p_2} + \frac{-ab}{a+b+p_3} + \cdots$$

where $a = e^{2\pi i x/n}$ and $b = e^{2\pi i y/n}$ with $0 \le x < y < n$ and $\gcd(y - x, n) = 1$. Verify that if $\sum_k |p_k| < \infty$, then for each $0 \le i < n$ there exists complex constants A_i and B_i such that

$$\lim_{k\to\infty} P_{nk+i} = A_i, \qquad \lim_{k\to\infty} Q_{nk+i} = B_i,$$

and evaluate, for each pair (i, j), the difference

$$A_i B_j - B_i A_j$$

in terms of a and b.

79. **A dense continued fraction**. Consider the continued fraction

$$c := \tfrac{4}{3} \; \underset{-}{} \; \tfrac{1}{4/3} \; \underset{-}{} \; \tfrac{1}{4/3} \; \underset{-}{} \ldots$$

and let $\{x_n\}$ be its sequence of convergents. Let S denote the set $\{x_n : 1 \leq n < \infty\}$. Plot the points of S on the real line. Prove that c does not converge and that in fact S is dense in $\mathbb{R}$ [83].

80. **Counting.** For a compelling general essay on the difficulty of applying advanced mathematical propositions to everyday life, we recommend "Why counting is impossible" [124, Chapter 7]. We add that according to *Today* (October 17, 2006), "The [U.S.] nation's population officially hit 300 million at 7:46 a.m. EDT." The source article at `http://www.msnbc.msn.com/id/15298443` concludes:

> "The census clearly misses people," said Passel, a former Census Bureau employee who used to help estimate the undercount. "Having said that, when they crossed 200 million, they were missing about 5 million people. We think the 2000 census missed a lot less than 5 million people."

81. **Intuition on the extremes.** Two very different recent books make the same point; as humans, we are very poor at making estimates of or preparations for highly unlikely events—be it the crash of 1929, 9/11, or two Katrina-like storms in one season—or of finding common sense on scales we have not evolved (á la Dawkins) to encompass— whether subatomic or astronomic. In *Faust in Copenhagen* [255, p. 152], Segré writes of the history of the Copenhagen interpretation of quantum mechanics:

> Because atomic behavior is so unlike ordinary experience, it is very difficult to get used to and appears peculiar and mysterious to everyone, both to the novice and to the experienced physicist. Even the experts do not understand it the way they would like to, and it is perfectly reasonable that they should not, because all of direct, human experience applies to large objects. We know how large objects will act, but things on a small scale just do not act that way. So we have to learn about them in a sort of abstract or imaginative fashion and not by connection with our direct human experience.

Of course, "large" for someone like Richard Feynman means a boulder, not the whole universe. Likewise, Taleb, in the *Black Swan: The*

Impact of the Highly Improbable [272] couches much of his argument around the difference between life in "Mediocristan" (Gaussian and predictable) and "Extremistan" (in which overgeneralization is eschewed, the counterfactual and the Mandelbrotian is celebrated, and his book sells orders of magnitude more than ours). Taleb argues that much decision making is consequently overquantified, irrelevant, and quite fatuous. On his web page `http://www.fooledbyrandomness.com`, he says, "My major hobby is teasing people who take themselves & the quality of their knowledge too seriously & those who don't have the guts to sometimes say: I don't know... ." Before the discovery of New Holland and Van Diemen's Land, a black swan was a European metaphor for the impossible.

Our methodology tries to mediate Popper and Taleb, Gauss and Mandelbrot.

82. **Kurt Gödel and the origins of computer science.** In a fascinating 2006 address sponsored by the Kurt Gödel Society, John W. Dawson[125] traces Gödel's views of and impact on computer science. Dawson makes reference to Gödel's 1951 *Gibbs Lectures* from which the quote on page 1 of this book is taken, and shows—along with much else—an unpublished 1956 letter to von Neumann. He finishes with the following questions:

   - If Gödel were alive today, what would he think of the role of computers in mathematics?
   - Would he approve of their use in providing numerical evidence for conjectures?
   - What would he think of computer-assisted proofs?
   - Would he maintain his belief in the mind's superiority?

83. **Five myths about artistic genius.** In Exercise 18 of Chapter 1, we discussed the nature of mathematical and scientific genius at some length. In the *Washington Post* article "Five Myths about Artistic Genius" (November 11, 2007), David Galenson, author of *Old Masters and Young Geniuses*, distinguishes between "precocious young geniuses" who "make bold and dramatic innovations" and "old masters" who "are experimental thinkers who proceed by trial and error." The article concludes "He is 56 years old and expects to do his best work in the future." So do we.

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Index of General Terms

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[3]In this Index, † denotes a quote.
[4]In this Index, ‡ denotes a figure.

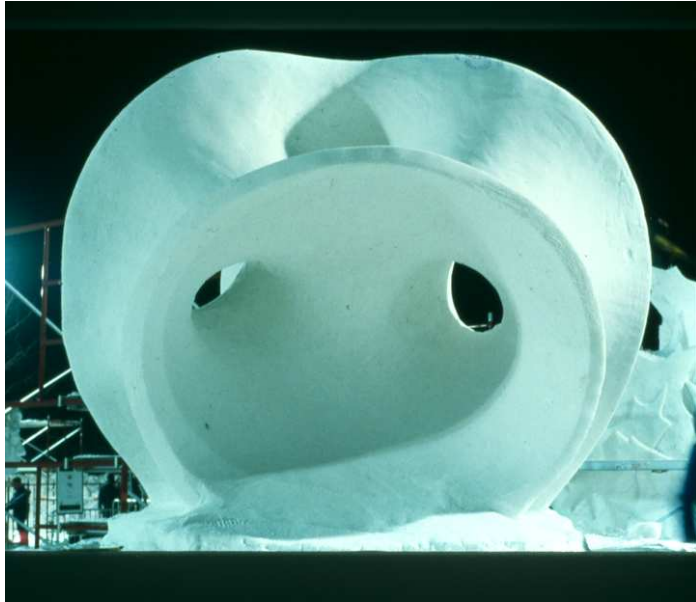Color Plate I. Pascal triangles modulo two? (See Figure 2.1).
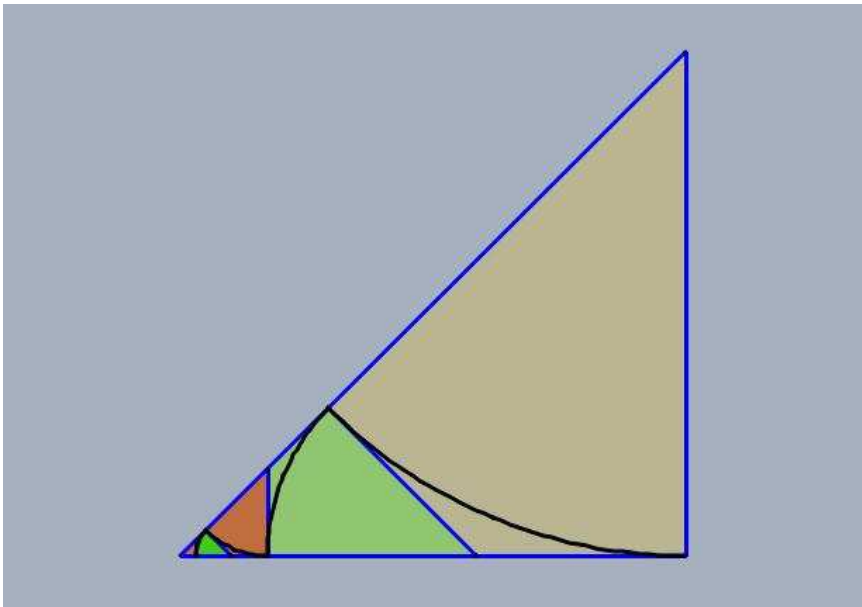
Color Plate II. Root two is irrational (See Figure 2.11).
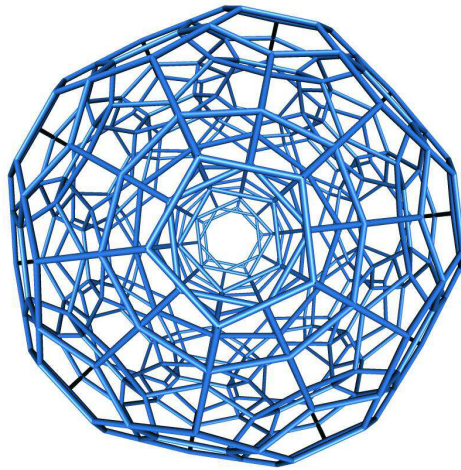
Color Plate III. Projection of 4-D polyhedron (See Figure 2.16).

Color Plate IV. Ferguson's "Eight-Fold Way" and "Figure-Eight Knot Complement" (See Figures 2.4 and 2.5).
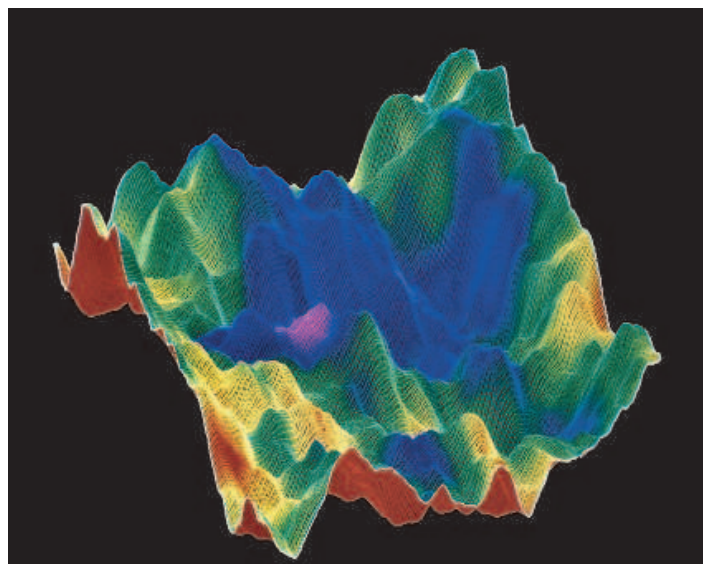
Color Plate V. Ferguson's "Invisible Handshake" (See Figure 2.17).

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 π (See Figure 4.1).