Mathematics by Experiment: Plausible Reasoning in the 21st Century
and
Experiments in Mathematics: Computational Paths to Discovery

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Preface

This document is an adapted selection of excerpts from two newly published books, *Mathematics by Experiment: Plausible Reasoning in the 21st Century*, and *Experimentation in Mathematics: Computational Paths to Discovery*, published by AK Peters, Natick, Massachussetts. We have gleaned from these two volumes material that explains what experimental mathematics is all about, as well as some of the more engaging examples of experimental mathematics in action.

The experimental methodology that we describe in these books 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. We have concentrated primarily on examples from analysis and number theory, but there are numerous excursions into other areas of mathematics as well. Much of this material is gleaned from existing sources, but there is a significant amount of material that, as far as we are aware, has not yet appeared in the literature.

Each of the two volumes is targeted to a fairly broad cross-section of mathematically trained readers. Most of the first 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. Some programming experience is useful, but not required.

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Chapters of the Two Volumes

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.expmath.info

Contents

Chapter 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

[*From Volume 1, Section 1.1*]

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 harness 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.

Perhaps the most important advancement in bringing mathematical research into the computer age 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 books are 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.

1.2 Proof versus Truth

[*From Volume 1, Sections 1.3*]

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.

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 [24]; (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 are described in greater detail in Volume 1, 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. 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 in Section 3.1) 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^{22}). 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.

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 (and in Section 4.2 of this document) 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.

1.3 Paradigm Shifts

[*From Volume 1, Section 1.4*]

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.

Jacques Hadamard (1865–1963) was perhaps the greatest mathematician to think deeply and seriously about cognition in mathematics. 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 [40])

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. [17, 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. [41, page 78]

1.4 Commentary and Additional Examples

[*From Volume 1, Chapter 1 Commentary*]

1. **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*.

   As this book was going to press, the *Annals of Mathematics* has decided to publish Hales' paper, but with a cautionary note, because although a team of referees is "99% certain" that the computer-assisted proof is sound, they have not been able to verify every detail [42]. One wonders if every other article in this journal has implicitly been certified to be correct with more than 99% certainty.

Chapter 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.

2.1 A Curious Anomaly in the Gregory Series

[*From Volume 1, Section 2.2*]

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

$$\pi \;=\; 4\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{2k-1} \;=\; 4(1-1/3+1/5-1/7+\cdots), \qquad (2.1.1)$$

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:

```
3.14159245358979323846464338327950278419716939938730582097494182230781640...
3.14159265358979323846264338327950288419716939937510582097494459230781640...
         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:

```
0.69314708055995530941723212125817656807551613436025525140068000949418722...
0.69314718055994530941723212145817656807550013436025525412068000949339362...
         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:

$$\begin{aligned}\sec x &= \sum_{k=0}^{\infty} \frac{(-1)^k E_{2k} x^{2k}}{(2k)!} \\ \tan x &= \sum_{k=0}^{\infty} \frac{(-1)^{k+1} T_{2k+1} x^{2k+1}}{(2k+1)!}.\end{aligned} \tag{2.1.2}$$

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:

$$\frac{\pi}{2} - 2\sum_{k=1}^{N/2} \frac{(-1)^{k+1}}{2k-1} \approx \sum_{m=0}^{\infty} \frac{E_{2m}}{N^{2m+1}} \tag{2.1.3}$$

$$\log 2 - \sum_{k=1}^{N/2} \frac{(-1)^{k+1}}{k} \approx \frac{1}{N} + \sum_{m=1}^{\infty} \frac{T_{2m-1}}{N^{2m}}. \tag{2.1.4}$$

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 (2.1.3) 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 [13] for proofs of (2.1.3) and (2.1.4), together with some additional details.)

2.2 Bifurcation Points in the Logistic Iteration

[*From Volume 1, Section 2.3*]

One of the classic examples of a chaotic iteration is known as the *logistic* iteration: Fix a real number $r > 0$, select x_0 in the unit interval $(0, 1)$, and then iterate

$$x_{k+1} = rx_k(1 - x_k). \tag{2.2.5}$$

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

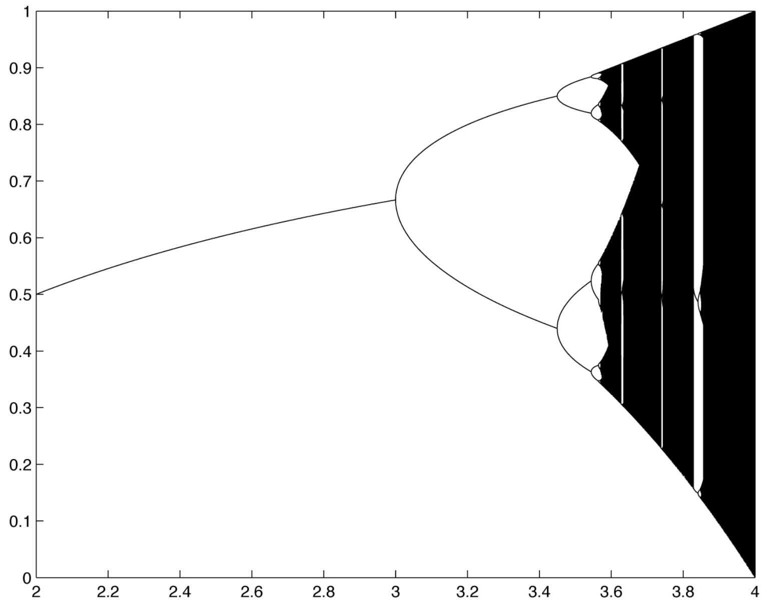

Figure 2.1: Bifurcation in the logistic iteration.

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 2.1.

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 (2.2.5), to demonstrate that this constant must be algebraic, but the bound on the degree of the integer polynomial that b_3 satisfies is quite large and thus not very useful.

A tool that can be used in such situations is an *integer relation algorithm*. This is an algorithm which, when given n real numbers $(x_1, x_2, \cdots, x_n)$, returns integers $(a_1, a_2, \cdots, a_n)$, not all zero, such that $a_1x_1 + a_2x_2 + \cdots + a_nx_n = 0$ (if such a solution exists). Such computations must be done using very high precision arithmetic, or else the results are not numerically significant. At present the best algorithm for integer relation detection appears to be the "PSLQ" algorithm of mathematician-sculptor Helaman Ferguson [30, 6, 8], although the "LLL" algorithm is also often used. We discuss integer relation detection in greater depth in Volume 1, Chapter 6. For the time being we mention the Internet-based integer relation tool at http://www.cecm.sfu.ca/projects/IntegerRelations and the Experimental Mathematician's Toolkit at http://www.expmath.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

$$
\begin{aligned}
0 \;=\; & 4913 + 2108t^2 - 604t^3 - 977t^4 + 8t^5 + 44t^6 + 392t^7 - 193t^8 - 40t^9 \\
& +48t^{10} - 12t^{11} + t^{12}. \qquad (2.2.6)
\end{aligned}
$$

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

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

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

```
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 [8]. The relation produced was recently verified by Konstantinos Karamanos, using the Magma computer algebra system [36].

2.3 Experimental Mathematics and Sculpture

[*From Volume 1, Section 2.4*]

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* [6]. 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 [29]. 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."

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 2.2, courtesy of Helaman Ferguson).

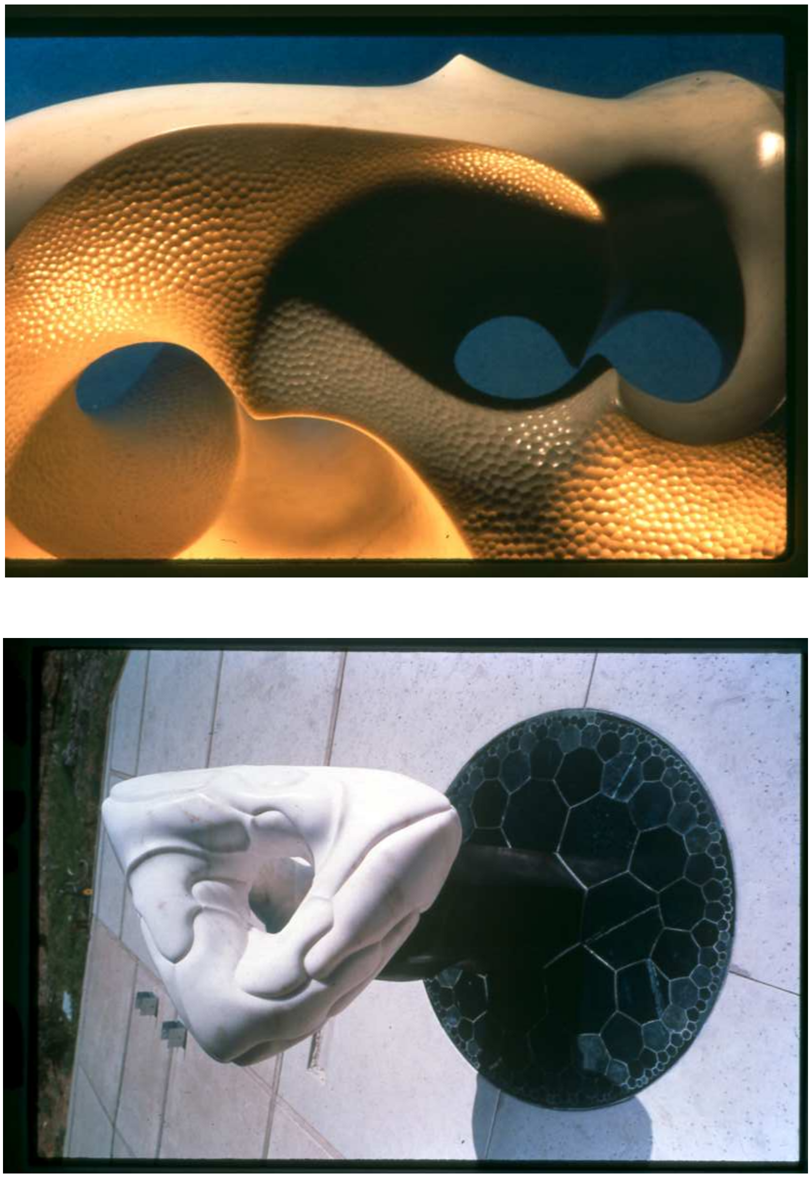

Figure 2.2: Ferguson's "Eight-Fold Way" and "Figure-Eight Knot Complement."

Another of Ferguson's well-known sculptures is the "Figure-Eight Complement II" (see Figure 2.2, courtesy of Helaman Ferguson). It has been known for some time that the hyperbolic volume V of the figure-eight knot complement is given by the formula

$$V = 2\sqrt{3}\sum_{n=1}^{\infty}\frac{1}{n\binom{2n}{n}}\sum_{k=n}^{2n-1}\frac{1}{k} \tag{2.3.7}$$

$$= 2.02988321281930725004240510854 9\ldots \tag{2.3.8}$$

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

$$C_j = \sum_{n=0}^{\infty}\frac{(-1)^n}{27^n(6n+j)^2}. \tag{2.3.9}$$

Indeed, it is, as Broadhurst [18] found using a PSLQ program:

$$V = \frac{\sqrt{3}}{9}\sum_{n=0}^{\infty}\frac{(-1)^n}{27^n}\left(\frac{18}{(6n+1)^2}-\frac{18}{(6n+2)^2}-\frac{24}{(6n+3)^2}\right.$$
$$\left.-\frac{6}{(6n+4)^2}+\frac{2}{(6n+5)^2}\right). \tag{2.3.10}$$

You can verify this yourself, using for example the Mathematician's Toolkit, available at http://www.expmath.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}]]
```

When this is done you will recover the solution vector $(9, -18, 18, 24, 6, -2, 0)$. A proof that formula (2.3.10) holds, together with a number of other identities for V, is given in the Volume 1, Section 2 Commentary.

As we shall see in Section 3.1, constants given by a formula of the general type given in (2.3.10), 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.

2.4 Recognition of Euler Sums

[*From Volume 1, Section 2.5*]

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 [11]

$$\begin{aligned} \sum_{k=1}^{\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^2 k^{-2} &= 4.59987\ldots \\ &\approx \frac{17}{4}\zeta(4) = \frac{17\pi^4}{360}. \end{aligned} \qquad (2.4.11)$$

The function $\zeta(s)$ in (2.4.11) is the classical *Riemann zeta function*,

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

Bernoulli showed that for even integers, $\zeta(2n)$ is a rational multiple of π^{2n} [15]. (Bernoulli's result is proved in Section 3.2 of the second volume of this work.)

Au-Yeung had computed the sum in (2.4.11) 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

$$\frac{1}{2\pi}\int_0^{\pi}(\pi-t)^2\log^2(2\sin\frac{t}{2})\,dt = \sum_{n=1}^{\infty}\frac{(\sum_{k=1}^{n}\frac{1}{k})^2}{(n+1)^2}. \qquad (2.4.12)$$

The idea here is that the series on the right of (2.4.12) permits one to evaluate (2.4.11), 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 [28]. 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

$$\sum_{k=1}^{\infty}\left(1+\frac{1}{2^m}+\cdots+\frac{1}{k^m}\right)(k+1)^{-n}. \tag{2.4.13}$$

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 $m = 1, n \geq 2$. Sums of this general form are nowadays known as "Euler sums" or "Euler-Zagier sums."

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 [12]. 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.

$$\begin{aligned}
\sum_{k=1}^{\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^2(k+1)^{-4} &= \frac{37}{22680}\pi^6-\zeta^2(3)\\
\sum_{k=1}^{\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^3(k+1)^{-6} &= \\
&\zeta^3(3)+\frac{197}{24}\zeta(9)+\frac{1}{2}\pi^2\zeta(7)-\frac{11}{120}\pi^4\zeta(5)-\frac{37}{7560}\pi^6\zeta(3)
\end{aligned}$$

$$\begin{aligned}
\sum_{k=1}^{\infty}\left(1-\frac{1}{2}+\cdots+(-1)^{k+1}\frac{1}{k}\right)^2(k+1)^{-3} &= \\
&4\,\mathrm{Li}_5\left(\frac{1}{2}\right)-\frac{1}{30}\log^5(2)-\frac{17}{32}\zeta(5)-\frac{11}{720}\pi^4\log(2)+\frac{7}{4}\zeta(3)\log^2(2)\\
&+\frac{1}{18}\pi^2\log^3(2)-\frac{1}{8}\pi^2\zeta(3),
\end{aligned} \tag{2.4.14}$$

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

2.5 Quantum Field Theory

[*From Volume 1, Section 2.6*]

In another recent development, David Broadhurst (who discovered the identity (2.3.10) 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 [19, 20]. 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 [18], 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 four-dimensional iterated integral, such as

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

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

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

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 2.3. 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 $C = \sum_{k>0}\sin(\pi k/3)/k^2$.

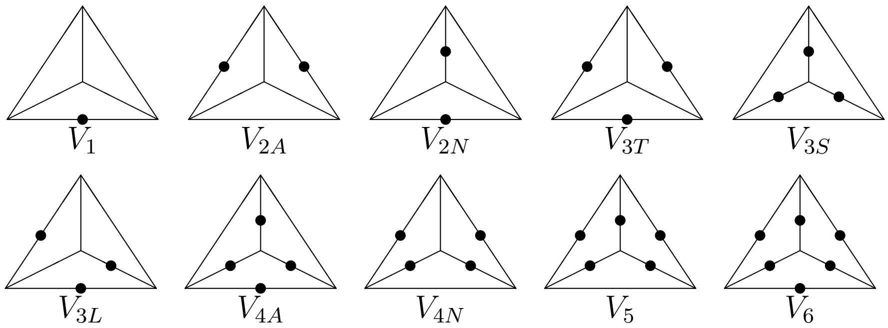

Figure 2.3: The ten tetrahedral configurations.

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

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

2.6 Definite Integrals and Infinite Series

[*From Volume 1, Section 2.7*]

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 following three integrals to over 100 decimal digit accuracy:

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

$$0.18067126259065494279230812898167161533711457101829676626624079429375856622413300177089825415048379970774 0\ldots$$

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

$$0.84351184168503463400262005199952815165168908642144429369711259690658735566923993839932791559637134802397 6\ldots \tag{2.6.15}$$

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

$$2.46740110027233965470862274996903778382842485181019765660333734405501120560480131075044335092963805795600 6\ldots \quad (2.6.16)$$

(the third of these is from [32]). Both *Maple* and *Mathematica* attempt to evaluate these definite integrals analytically. In each case, however, while the results appear to be technically correct, they are not very useful, in that they are either rather lengthy, or involve advanced functions and complex entities. We suspect that there are considerably simpler closed-form versions.

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

$$\begin{aligned}
\int_0^1 \frac{t^2 \log(t)\, dt}{(t^2-1)(t^4+1)} &= \frac{\pi^2(2-\sqrt{2})}{32} \\
\int_0^{\pi/4} \frac{t^2\, dt}{\sin^2(t)} &= -\frac{\pi^2}{16} + \frac{\pi \log(2)}{4} + G \\
\int_0^\pi \frac{x \sin x \, dx}{1+\cos^2 x} &= \frac{\pi^2}{4},
\end{aligned} \quad (2.6.17)$$

where G denotes Catalan's constant

$$G = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2}.$$

2.7 Commentary and Additional Examples

[*From Volume 1, Chapter 2 Commentary*]

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

$$\sigma = \sqrt[8]{2207 - \cfrac{1}{2207 - \cfrac{1}{2207 - \cfrac{1}{2207 - \cdots}}}}. \quad (2.7.18)$$

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: $(3 + \sqrt{5})/2$.

2. **Two radical expressions.** (From [34, 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 $\sqrt[3]{\frac{3}{2}\sqrt[3]{9} - 3}$.

3. **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 2.4 now resides at York University in Toronto.

   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."

   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 2.5.

Figure 2.4: Donald Coxeter's own kaleidoscope

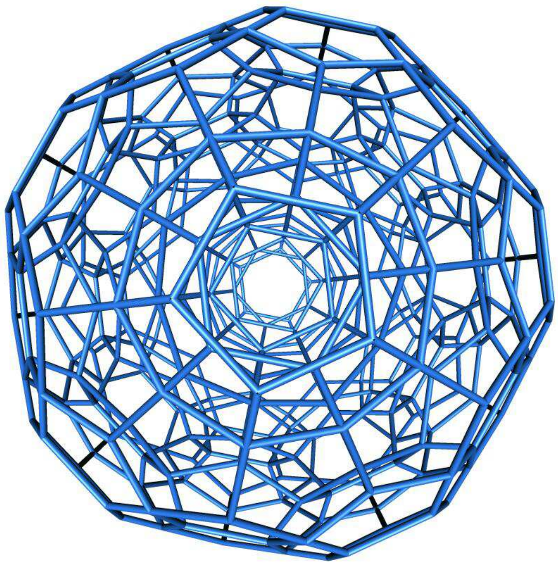

Figure 2.5: A projection of a four dimensional polytope.

Chapter 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.

3.1 Computing Individual Digits of Pi

[*From Volume 1, Section 3.4*]

An outsider might be forgiven for thinking that essentially everything of interest with regards to π has been discovered. 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 [7]. 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 2001-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 3.1.1

$$\pi \;=\; \sum_{i=0}^{\infty} \frac{1}{16^i}\left(\frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6}\right). \tag{3.1.1}$$

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

$$\begin{aligned}\int_0^{1/\sqrt{2}} \frac{x^{k-1}}{1-x^8}\,dx \;&=\; \int_0^{1/\sqrt{2}} \sum_{i=0}^{\infty} x^{k-1+8i}\,dx \\ &=\; \frac{1}{2^{k/2}} \sum_{i=0}^{\infty} \frac{1}{16^i(8i+k)}.\end{aligned} \tag{3.1.2}$$

Thus one can write

$$\begin{aligned}&\sum_{i=0}^{\infty} \frac{1}{16^i}\left(\frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6}\right) \\ &\quad= \int_0^{1/\sqrt{2}} \frac{4\sqrt{2} - 8x^3 - 4\sqrt{2}x^4 - 8x^5}{1-x^8}\,dx,\end{aligned} \tag{3.1.3}$$

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

$$\begin{aligned}\int_0^1 \frac{16\,y - 16}{y^4 - 2\,y^3 + 4\,y - 4}\,dy &= \int_0^1 \frac{4y}{y^2-2}\,dy - \int_0^1 \frac{4y-8}{y^2-2y+2}\,dy \\ &= \pi. \end{aligned} \tag{3.1.4}$$

□

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

It all began in 1995, when Peter Borwein and Simon Plouffe of Simon Fraser University observed that the following well-known formula for log 2 permits one to calculate isolated digits in the binary expansion of log 2:

$$\log 2 = \sum_{k=0}^{\infty} \frac{1}{k2^k}. \tag{3.1.5}$$

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

$$\begin{aligned}\{2^d \log 2\} &= \left\{\left\{\sum_{k=0}^{d} \frac{2^{d-k}}{k}\right\} + \sum_{k=d+1}^{\infty} \frac{2^{d-k}}{k}\right\} \\ &= \left\{\left\{\sum_{k=0}^{d} \frac{2^{d-k} \bmod k}{k}\right\} + \sum_{k=d+1}^{\infty} \frac{2^{d-k}}{k}\right\}. \end{aligned} \tag{3.1.6}$$

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 (3.1.6), 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 [35, pg. 461]. In our application, we need to obtain the exponentiation result modulo a positive integer k. This can be done very efficiently as follows:

Algorithm 1 *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 $r \leftarrow br \bmod k$; $n \leftarrow n - t$; endif
$t \leftarrow t/2$
if $t \geq 1$ then $r \leftarrow r^2 \bmod k$; go to A; endif ☐

Note that the above algorithm is performed entirely with positive integers that do not exceed k^2 in size. Thus ordinary 64-bit floating-point or integer arithmetic, available on almost all modern computers, suffices for even rather large calculations. 128-bit floating-point arithmetic (double-double or quad precision), available at least in software on many systems (see Volume 1, Section 6.2), suffices for the largest computations currently feasible.

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

Algorithm 2 *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 (3.1.6), using Algorithm 1, implemented using ordinary 64-bit integer or 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

$$\alpha = \sum_{k=0}^{\infty} \frac{p(k)}{q(k)2^k}, \tag{3.1.7}$$

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 (3.1.7).

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 [30, 5]. We discuss the PSLQ algorithm and related techniques more in Volume 1, 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 $(\alpha_i,\ 2 \le i \le n)$ 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 (3.1.1) was finally uncovered. The actual formula found by the computation was:

$$\pi = 4F(1/4, 5/4; 1; -1/4) + 2\arctan(1/2) - \log 5, \tag{3.1.8}$$

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:

$$\pi = \sum_{i=0}^{\infty} \frac{1}{16^i} \left(\frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6} \right). \tag{3.1.9}$$

It should be clear at this point that the scheme for computing individual hexadecimal digits of π is very similar to Algorithm 2. For completeness, we state it as follows:

Algorithm 3 *Individual digit algorithm for π.*

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

$$\{16^d \pi\} = \{4\{16^d S_1\} - 2\{16^d S_4\} - \{16^d S_5\} - \{16^d S_6\}\}, \tag{3.1.10}$$

where

$$S_j = \sum_{k=0}^{\infty} \frac{1}{16^k(8k+j)}. \tag{3.1.11}$$

Now apply Algorithm 2, with

$$\begin{aligned} \{16^d S_j\} &= \left\{ \left\{ \sum_{k=0}^{d} \frac{16^{d-k}}{8k+j} \right\} + \sum_{k=d+1}^{\infty} \frac{16^{d-k}}{8k+j} \right\} \\ &= \left\{ \left\{ \sum_{k=0}^{d} \frac{16^{d-k} \bmod 8k+j}{8k+j} \right\} + \sum_{k=d+1}^{\infty} \frac{16^{d-k}}{8k+j} \right\} \end{aligned} \tag{3.1.12}$$

instead of equation (3.1.6), to compute $\{16^d S_j\}$ for $j = 1, 4, 5, 6$. Combine these four results, discarding integer parts, as shown in (3.1.10). The resulting fraction, when expressed in hexadecimal notation, gives the hex digit of π in position $d+1$, plus a few more correct digits. □

As with Algorithm 2, 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 [7]. Sample implementations in both C and Fortran-90 are available from the web site http://www.expmath.info.

Needless to say, Algorithm 3 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

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 3.1: Computed hexadecimal digits of π.

workstations working in parallel over the Internet. His scheme is actually based on the following variant of 3.1.9:

$$\begin{aligned} \pi &= 4\sum_{k=0}^{\infty} \frac{(-1)^k}{4^k(2k+1)} \\ &\quad -\frac{1}{64}\sum_{k=0}^{\infty} \frac{(-1)^k}{1024^k}\left(\frac{32}{4k+1}+\frac{8}{4k+2}+\frac{1}{4k+3}\right). \end{aligned} \tag{3.1.13}$$

This formula permits individual hex or binary digits of π to be calculated roughly 43% faster than (3.1.1).

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 3.1 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 Volume 1, Section 3.7) [14].

3.2 Commentary and Additional Examples

[*From Volume 1, Chapter 3 Commentary*]

1. **An arctan series for pi.** Find rational coefficients a_i such that the identity

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

holds [3, 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 Volume 1, Section 6.3), or try the tools at one of these sites: http://www.cecm.sfu.ca/projects/IntegerRelations or http://www.expmath.info.

2. **Biblical pi.** 1 Kings 7:23 and 2 Chronicles 4:2 describe a circular pool in Solomon's temple "ten cubits from brim to brim," and 30 cubits in circumference, so that $\pi = 3$. In spite of the clearly informal context, 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 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 [9, pg. 75–76].

Chapter 4

Sequences, Series, Products and Integrals

> Several years ago I was invited to contemplate being marooned on the proverbial desert island. What book would I most wish to have there, in addition to the Bible and the complete works of Shakespeare? My immediate answer was: Abramowitz and Stegun's *Handbook of Mathematical Functions*. If I could substitute for the Bible, I would choose Gradsteyn and Ryzhik's *Table of Integrals, Series and Products*. Compounding the impiety, I would give up Shakespeare in favor of Prudnikov, Brychkov and Marichev's *Tables of Integrals and Series*... On the island, there would be much time to think about waves on the water that carve ridges on the sand beneath and focus sunlight there; shapes of clouds; subtle tints in the sky... With the arrogance that keeps us theorists going, I harbor the delusion that it would be not too difficult to guess the underlying physics and formulate the governing equations. It is when contemplating how to solve these equations—to convert formulations into explanations—that humility sets in. Then, compendia of formulas become indispensable.
>
> Michael Berry, "Why Are Special Functions Special?", 2001

In the first volume, we presented numerous examples of experimental mathematics in action. In particular, we examined how a computational-experimental approach could be used to identify constants and sequences, evaluate definite integrals and infinite series, discover new identities involving fundamental constants and functions of mathematics, provide a more intuitive approach to mathematical proofs, and formulate conjectures that can lead to important advances in the field. In this chapter, we introduce our discussion with a number of additional intriguing examples in the realm of sequences, series, products and integrals.

4.1 Pi Is Not 22/7

[*From Volume 2, Section 1.1*]

We first consider an example from the early history of π, as described in Chapter 3 of the first volume.

Even *Maple* or *Mathematica* "knows" $\pi \neq 22/7$, since

$$0 \quad < \quad \int_0^1 \frac{(1-x)^4 x^4}{1+x^2}\, dx \quad = \quad \frac{22}{7} - \pi, \tag{4.1.1}$$

though it would be prudent to ask "why" it can perform the evaluation and "whether" we should trust it?

Assume we trust it. Then the integrand is strictly positive on the interior of the interval of integration, and the answer in (4.1.1) is necessarily an area and thus strictly positive, despite millennia of claims that π is 22/7. Of course, 22/7 is one of the early continued fraction approximations to π. The first four are $3, 22/7, 333/106, 355/113$.

In this case, computing the indefinite integral provides immediate reassurance. We obtain

$$\int_0^t \frac{x^4\,(1-x)^4}{1+x^2}\, dx \quad = \quad \frac{1}{7}\,t^7 - \frac{2}{3}\,t^6 + t^5 - \frac{4}{3}\,t^3 + 4\,t - 4\,\arctan(t)\,. \tag{4.1.2}$$

This is easily confirmed by differentiation, and the Fundamental Theorem of Calculus substantiates (4.1.1).

In fact, one can take this idea a bit further. We note that

$$\int_0^1 x^4\,(1-x)^4\, dx \quad = \quad \frac{1}{630}, \tag{4.1.3}$$

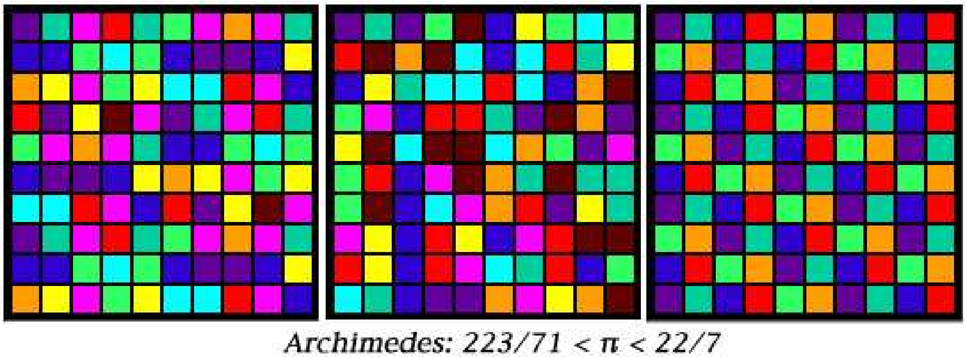

Figure 4.1: A pictorial proof of Archimedes' inequality

and we observe that

$$\frac{1}{2}\int_0^1 x^4\,(1-x)^4\,dx \quad < \quad \int_0^1 \frac{(1-x)^4x^4}{1+x^2}\,dx < \int_0^1 x^4\,(1-x)^4\,dx. \quad (4.1.4)$$

On combining this with (4.1.1) and (4.1.3), we straightforwardly derive $223/71 < 22/7 - 1/630 < \pi < 22/7 - 1/1260 < 22/7$, and so re-obtain Archimedes' famous computation

$$3\frac{10}{71} < \pi < 3\frac{10}{70} \quad (4.1.5)$$

(illustrating that it is sometimes better not to fully reduce a fraction to lowest terms).

This derivation of the estimate above seems first to have been written down in *Eureka*, the Cambridge student journal in 1971 [25]. The integral in (4.1.1) was apparently shown by Kurt Mahler to his students in the mid-1960s, and it had appeared in a mathematical examination at the University of Sydney in November, 1960. Figure 4.1 (also in the Color Supplement) shows the estimate graphically illustrated. The three 10×10 arrays color the digits of the first hundred digits of 223/71, π, and 22/7. One sees a clear pattern on the right (22/7), a more subtle structure on the left (223/71), and a "random" coloring in the middle (π).

It is tempting to ask if there is a clean general way to mimic (4.1.1) for more general rational approximations, or even continued fraction convergents. This is indeed possible to some degree, as discussed by Beukers in [10]. The most satisfactory result is

$$a_n\pi - \frac{b_n}{c_n} = \int_0^1 \frac{t^{2n}\left(1-t^2\right)^{2n}\left(\left(1+it\right)^{3n+1}+\left(1-it\right)^{3n+1}\right)}{\left(1+t^2\right)^{3n+1}}dt, \qquad (4.1.6)$$

for $n \geq 1$, where the integers a_n, b_n and c_n are implicitly defined by the integral in (4.1.6). The first three integrals evaluate to $14\pi - 44$, $968\pi - 45616/15$, and $75920\pi - 1669568/7$, so again we start with $\pi - 22/7$.

Unlike Beukers' preliminary attempts in [10], such as the seemingly promising

$$\int_0^1 \frac{t^n\left(1-t\right)^n}{\left(t^2+1\right)^{n+1}}dt,$$

this set of approximates actually produces an explicit if weak *irrationality estimate* [15, 10]: for large n,

$$\left|\pi - \frac{p_n}{q_n}\right| \geq \frac{1}{q_n^{1.0499}}.$$

As Beukers sketches, one consequence of this explicit sequence

$$\left|\pi - \frac{p}{q}\right| \geq \frac{1}{q^{21.04\ldots}}$$

for all integers p, q with sufficiently large q. (Here $21.04\ldots = 1 + 1/0.0499$. In fact, in 1993 Hata by different methods had improved the number 21.4 to 8.02.)

While it is easy to discover "natural" results like

$$\frac{1}{5}\int_0^1 \frac{x\left(1-x\right)^2}{\left(1+x\right)^3}\,dx = \frac{7}{10} - \log\left(2\right), \qquad (4.1.7)$$

the fact that 7/10 is again a convergent to $\log 2$ seems to be largely a happenstance. For example,

$$\begin{aligned}
\int_0^1 \frac{x^{12}\left(1-x\right)^{12}}{16\left(1+x^2\right)}\,dx &= \frac{431302721}{137287920} - \pi \\
\int_0^1 \frac{x^{12}\left(1-x\right)^{12}}{16}\,dx &= \frac{1}{1081662400}
\end{aligned}$$

leads to the true, if inelegant, estimate that $5902037233/1878676800 < \pi < 224277414953/71389718400$, where the interval is of size $1.39 \cdot 10^{-9}$.

4.2 High Precision Fraud

[*From Volume 2, Section 1.4*]

Consider the sums

$$\sum_{n=1}^{\infty} \frac{\lfloor n \tanh(\pi) \rfloor}{10^n} \stackrel{?}{=} \frac{1}{81},$$

an evaluation that is wrong, but valid to 268 decimal places, and

$$\sum_{n=1}^{\infty} \frac{\lfloor n \tanh(\pi/2) \rfloor}{10^n} \stackrel{?}{=} \frac{1}{81},$$

which is valid to "only" 12 places. Both series actually evaluate to transcendental numbers.

What underlies these "fraudulent" evaluations? The "quick" reason is that $\tanh(\pi)$ and $\tanh(\pi/2)$ are almost integers, with, e.g., $0.99 < \tanh(\pi) < 1$. Therefore, $\lfloor n \tanh(\pi) \rfloor$ will be equal to $n-1$ for many n; precisely for $n = 1, \cdots, 268$. Since

$$\sum_{n=1}^{\infty} \frac{n-1}{10^n} = \frac{1}{81},$$

this explains the evaluations. Looking more closely at this argument, one is directly led to *continued fractions* as the deeper reason behind the frauds. For any irrational positive α, we can write

$$\begin{aligned} \alpha &= [a_0, a_1, \cdots, a_n, a_{n+1}, \cdots] \\ &= a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \cdots}}}, \end{aligned}$$

with integral a_n and $a_0 \geq 0$, $a_n \geq 1$ for $n \geq 1$. This is hard to compute by hand, but easy even on a small computer or calculator. For the parameters in our series, we get

$$\tanh(\pi) = [0, 1, \mathbf{267}, 4, 14, 1, 2, 1, 2, 2, 1, 2, 3, 8, 3, 1, \cdots] \tag{4.2.8}$$

and

$$\tanh\left(\frac{\pi}{2}\right) = [0, 1, \mathbf{11}, 14, 4, 1, 1, 1, 3, 1, 295, 4, 4, 1, 5, 17, 7, \cdots]. \tag{4.2.9}$$

It cannot be a coincidence that the integers 267 and 11 (each equal to the number of places of agreement with 1/81 in the respective formula) appear in these expansions! There must be a connection between series of the type $\sum \lfloor n\alpha \rfloor z^n$ and the continued fraction expansion of an irrational α. In fact, consider the infinite continued fraction approximations for α generated by

$$\begin{aligned} p_{n+1} &= p_n a_{n+1} + p_{n-1}, \qquad p_0 = a_0 = \lfloor \alpha \rfloor, \qquad p_{-1} = 1, \\ q_{n+1} &= q_n a_{n+1} + q_{n-1}, \qquad q_0 = 1, \qquad q_{-1} = 0. \end{aligned}$$

Then for $n \geq 0$, p_{2n}/q_{2n} increases to α, while p_{2n+1}/q_{2n+1} decreases to α and

$$\frac{1}{q_n\left(q_n + q_{n+1}\right)} < \left|\alpha - \frac{p_n}{q_n}\right| < \frac{1}{q_n\, q_{n+1}}.$$

Let further $\epsilon_n = q_n\alpha - p_n$. Then from the above, it follows that

$$|\epsilon_{n+1}| < \frac{1}{q_n + q_{n+1}} < |\epsilon_n| < \frac{1}{q_{n+1}} \leq 1.$$

All of this is standard and may be found in [33], [43], or [39]. Our aim now is to show a relationship between the above series and the continued fraction expansion of α. A first key is the following lemma, which we will not prove here since it requires some knowledge about linear Diophantine equations (see [16], from which this material is taken).

Lemma 4.2.1 *For any irrational $\alpha > 0$ and $n, N \in \mathrm{N}$, we have*

$$\begin{aligned} \lfloor n\alpha + \epsilon_N \rfloor &= \lfloor n\alpha \rfloor && \text{for } n < q_{N+1}, \\ \lfloor n\alpha + \epsilon_N \rfloor &= \lfloor n\alpha \rfloor + (-1)^N && \text{for } n = q_{N+1}. \end{aligned}$$

Theorem 4.2.2 *For irrational $\alpha > 0$,*

$$\sum_{n=1}^{\infty} \lfloor n\alpha \rfloor z^n = \frac{p_0\, z}{(1-z)^2} + \sum_{n=0}^{\infty} (-1)^n \frac{z^{q_n} z^{q_{n+1}}}{\left(1 - z^{q_n}\right)\left(1 - z^{q_{n+1}}\right)}.$$

Proof. Let

$$G_\alpha(z,w) = \sum_{n=1}^{\infty} z^n\, w^{\lfloor n\alpha \rfloor}, \tag{4.2.10}$$

for $|z|, |w| < 1$. Then for $N > 0$,

$$\begin{aligned}
(1 - z^{q_N} w^{p_N})\, G_\alpha(z,w) - \sum_{n=1}^{q_N} z^n w^{\lfloor n\alpha \rfloor} \\
&= \sum_{n=1}^{\infty} z^{n+q_N} \left(w^{\lfloor (n+q_N)\alpha \rfloor} - w^{\lfloor n\alpha \rfloor + p_N} \right) \\
&= \sum_{n=1}^{\infty} z^{n+q_N} w^{\lfloor n\alpha \rfloor + p_N} \left(w^{\lfloor n\alpha + \epsilon_N \rfloor - \lfloor n\alpha \rfloor} - 1 \right) \\
&= z^{q_{N+1}+q_N} w^{\lfloor q_{N+1}\, \alpha \rfloor + p_N} \left(w^{(-1)^N} - 1 \right) + O(z^{q_{N+1}+q_N+1}) \\
&= z^{q_{N+1}+q_N} w^{p_{N+1}+p_N} (-1)^N \, \frac{w-1}{w} + O(z^{q_{N+1}+q_N+1}),
\end{aligned} \tag{4.2.11}$$

since $\lfloor q_{N+1}\alpha \rfloor = \lfloor \epsilon_{N+1} \rfloor + p_{N+1} = p_{N+1}$ if N is odd, and $= p_{N+1} - 1$ if N is even.

Now write $P_N = \sum_{n=1}^{q_N} z^n\, w^{\lfloor n\alpha \rfloor}$ and $Q_N = 1 - z^{q_N} w^{p_N}$. Then $A_N = Q_N P_{N+1} - Q_{N+1} P_N$ is a polynomial of degree at most $q_N + q_{N+1}$ in z, and therefore it follows from (4.2.11) that

$$\begin{aligned}
A_N &= Q_{N+1}(Q_N G_\alpha - P_N) - Q_N(Q_{N+1} G_\alpha - P_{N+1}) \\
&= (-1)^N \, \frac{w-1}{w} z^{q_N} w^{p_N} z^{q_{N+1}} w^{p_{N+1}}.
\end{aligned}$$

This in turn implies

$$\frac{P_{N+1}}{Q_{N+1}} - \frac{P_N}{Q_N} = \frac{A_N}{Q_N Q_{N+1}} = (-1)^N \, \frac{w-1}{w} \frac{z^{q_N} w^{p_N} z^{q_{N+1}} w^{p_{N+1}}}{Q_N Q_{N+1}}.$$

Next summing from zero to infinity, and noting that (4.2.11) implies that $G_\alpha - P_N/Q_N$ tends to 0 as N tends to infinity, shows that

$$G_\alpha(z,w) = \frac{z w^{p_0}}{1 - z w^{p_0}} - \frac{1-w}{w} \sum_{n=0}^{\infty} (-1)^n \frac{z^{q_n} w^{p_n} z^{q_{n+1}} w^{p_{n+1}}}{(1 - z^{q_n} w^{p_n})\,(1 - z^{q_{n+1}} w^{p_{n+1}})}.$$

Now differentiating with respect to w and then letting w tend to 1 proves the assertion. □

This theorem was first proved (for $\alpha \in (0,1)$) by Mahler in [37].

Example 4.2.3 $\alpha = \tanh(\pi)$.

In this case, $q_n = 1, 1, 268, 1073, \cdots$ for $n = 0, 1, 2, 3, \cdots$, and thus

$$\sum_{n=1}^{\infty} \lfloor n \tanh(\pi) \rfloor z^n \;=\; \frac{z^2}{(1-z)^2} - \frac{z^{269}}{(1-z)(1-z^{268})} + \cdots .$$

Therefore,

$$\frac{1}{81} - 2\cdot 10^{-269} \;\le\; \sum_{n=1}^{\infty} \frac{\lfloor n \tanh(\pi) \rfloor}{10^n} \;\le\; \frac{1}{81} + 2\cdot 10^{-269},$$

and similarly for $\alpha = \tanh(\frac{\pi}{2})$. □

Example 4.2.4 $\alpha = e^{\pi\sqrt{163/9}}$.

With one of our favorite transcendental numbers, $\alpha = e^{\pi\sqrt{163/9}} = [640320, 1653264929, \cdots]$, we get the incorrect evaluation

$$\sum_{n=1}^{\infty} \frac{\lfloor n e^{\pi\sqrt{163/9}} \rfloor}{2^n} \;\stackrel{?}{=}\; 1280640,$$

which is, however, correct to at least half a billion digits. □

4.3 Knuth's Series Problem

[*From Volume 2, Section 1.5*]

We give an account here of the solution, by one of the present authors (Borwein) to a problem recently posed by Donald E. Knuth of Stanford University in the *American Mathematical Monthly* (Problem 10832, Nov. 2000):

Problem: Evaluate

$$S = \sum_{k=1}^{\infty} \left(\frac{k^k}{k! e^k} - \frac{1}{\sqrt{2\pi k}} \right).$$

Solution: We first attempted to obtain a numerical value for S. Using *Maple*, we produced the approximation

$$S \approx -0.08406950872765599646.$$

Based on this numerical value, the Inverse Symbolic Calculator, available at the URL http://www.cecm.sfu.ca/projects/ISC, with the "Smart Lookup" feature, yielded the result

$$S \approx -\frac{2}{3} - \frac{1}{\sqrt{2\pi}} \zeta\left(\frac{1}{2}\right). \tag{4.3.12}$$

Calculations to even higher precision (50 decimal digits) confirmed this approximation. Thus within a few minutes we "knew" the answer.

Why should such an identity hold? One clue was provided by the surprising speed with which *Maple* was able to calculate a high-precision value of this slowly convergent infinite sum. Evidently, the *Maple* software knew something that we did not. Peering under the covers, we found that *Maple* was using the Lambert W function, which is the functional inverse of $w(z) = ze^z$.

Another clue was the appearance of $\zeta(1/2)$ in the above experimental identity, together with an obvious allusion to Stirling's formula in the original problem. This led us to conjecture the identity

$$\sum_{k=1}^{\infty} \left(\frac{1}{\sqrt{2\pi k}} - \frac{P(1/2, k-1)}{(k-1)!\sqrt{2}} \right) = \frac{1}{\sqrt{2\pi}} \zeta\left(\frac{1}{2}\right), \tag{4.3.13}$$

where $P(x, n)$ denotes the Pochhammer function $x(x+1)\cdots(x+n-1)$, and where the binomial coefficients in the LHS of (4.3.13) are the same as those of the function $1/\sqrt{2-2x}$. *Maple* successfully evaluated this summation, as shown on the RHS. We now needed to establish that

$$\sum_{k=1}^{\infty} \left(\frac{k^k}{k! e^k} - \frac{P(1/2, k-1)}{(k-1)!\sqrt{2}} \right) = -\frac{2}{3}.$$

Guided by the presence of the Lambert W function

$$W(z) \;=\; \sum_{k=1}^{\infty} \frac{(-k)^{k-1} z^k}{k!},$$

an appeal to Abel's limit theorem suggested the conjectured identity

$$\lim_{z \to 1} \left(\frac{dW(-z/e)}{dz} + \frac{1}{2 - 2z} \right) \;=\; 2/3.$$

Here again, *Maple* was able to evaluate this summation and establish the identity. □

4.4 Commentary and Additional Examples

[*From Volume 2, Chapter 1 Commentary*]

1. **Putnam problem 1999–A3.** Consider the power series expansion

$$\frac{1}{1 - 2x - x^2} = \sum_{n \geq 0} a_n x^n.$$

Prove that for each integer $n \geq 0$, there is an integer m such that

$$a_n^2 + a_{n+1}^2 = a_m.$$

Answer: It transpires that

$$a_n^2 + a_{n+1}^2 = a_{2n+1}, \tag{4.4.14}$$

which remains to be proven. Hint: The first 15 coefficients are

$$1, 2, 5, 12, 29, 70, 169, 408, 985, 2378, 5741, 13860, 33461, 80782, 195025,$$

and the desired squares are

$$5, 29, 169, 985, 5741, 33461, 195025,$$

which is more than enough to spot the pattern. To prove this either explicitly use the closed form for

$$a_n = \frac{1}{2\sqrt{2}}\left(\left(1+\sqrt{2}\right)^{n+1} - \left(-\sqrt{2}+1\right)^{n+1}\right),$$

or show that both sides of (4.4.14) satisfy the same recursion (and initial conditions).

2. **Putnam problem 2000–A4.** Show that the improper integral

$$\mathcal{I} = \lim_{M\to\infty} \int_0^M \sin(x)\sin(x^2)\,dx \tag{4.4.15}$$

exists. Hint: Numerical experimentation shows that a limit of approximately 0.4917 is reached. The existence of the limit can be rigorously established in two ways:

(a) Since the integrand equals $\cos(x^2-x)-\cos(x^2+x))/2$, it suffices to show that $\lim_{M\to\infty}\int_0^M \cos(x+x^2)\,dx$ exists. After a change of variables, it suffices to consider

$$\sum_{k=0}^{n-1}\int_{(k-1/2)\pi}^{(k+1/2)\pi} \frac{\cos(u)}{\sqrt{1+4\,u}}\,du.$$

This converges by the alternating series test.

(b) Use Cauchy's theorem to integrate the entire functions $\exp(ix^2 \pm ix)$ over a triangular path with vertices at $0, M$ and $(1+i)M$. Easy estimates show that the integrals over the vertical and the diagonal edges converge.

3. **Two expected distances.** These results originate with James D. Klein.

   (a) The expected distance between two random points on different sides of the unit square:

$$\begin{aligned}
&\frac{2}{3}\int_0^1\int_0^1 \sqrt{x^2+y^2}\,dx\,dy + \frac{1}{3}\int_0^1\int_0^1 \sqrt{1+(y-u)^2}\,du\,dy \\
=\ & 0.86900905527453446388497059434540662485671 9\ldots \\
=\ & \frac{2}{9}+\frac{1}{9}\sqrt{2}+\frac{5}{9}\log\left(1+\sqrt{2}\right).
\end{aligned}$$

(b) The expected distance between two random points on different faces of the unit cube:

$$\begin{aligned}
& \frac{4}{5}\int_0^1\int_0^1\int_0^1\int_0^1 \sqrt{x^2+y^2+(z-w)^2}\,dw\,dx\,dy\,dz \\
+ & \frac{1}{5}\int_0^1\int_0^1\int_0^1\int_0^1 \sqrt{1+(y-u)^2+(z-w)^2}\,du\,dw\,dy\,dz \\
= & \ 0.926390055174046729218163586547779014444960190107\,34\ldots \\
= & \ \frac{4}{75}+\frac{17}{75}\sqrt{2}-\frac{2}{25}\sqrt{3}-\frac{7}{75}\pi \\
& +\frac{7}{25}\log\left(1+\sqrt{2}\right)+\frac{7}{25}\log\left(7+4\sqrt{3}\right).
\end{aligned}$$

(c) Show that the first term in (b) is

$$\frac{\sqrt{2\pi}}{5}\sum_{n=2}^{\infty}\frac{\mathrm{F}\left(1/2,-n+2;3/2;1/2\right)}{(2\,n+1)\,\Gamma\left(n+2\right)\Gamma\left(5/2-n\right)}$$

$$+\frac{4}{15}\sqrt{2}+\frac{2}{5}\log\left(\sqrt{2}+1\right)-\frac{1}{75}\pi$$

and the second term is

$$\frac{\sqrt{\pi}}{10}\sum_{n=0}^{\infty}\frac{\mathrm{F}\left(1,1/2,-1/2-n,-n-1;2,1/2-n,3/2;-1\right)}{(2\,n+1)\,\Gamma\left(n+2\right)\Gamma\left(3/2-n\right)}$$

$$-\frac{2}{25}+\frac{\sqrt{2}}{50}+\frac{1}{10}\log\left(\sqrt{2}+1\right).$$

This allows one to numerically compute the expectation to high precision and to express both of the individual integrals in terms of the same set of constants. These expectations have actually been checked by computer simulations. Hint: Reduce the first integral to a three dimensional one, and use the binomial theorem on both.

Chapter 5

Partitions and Powers

> I'll be glad if I have succeeded in impressing the idea that it is not only pleasant to read at times the works of the old mathematical authors, but this may occasionally be of use for the actual advancement of science.
>
> Constantin Carathéodory, speaking to an MAA meeting in 1936

In this chapter, we address the theory of additive partitions and the theory of representations as sums of squares, both from an experimental perspective. Each has a distinguished history. We will show that computational techniques can accelerate both solution and understanding of these problems. What's more, these techniques have a number of interesting applications, including, for instance, Madelung's constant in physical chemistry.

5.1 Partition Functions

[*From Volume 2, Section 4.1*]

The number of *additive partitions* of n, $p(n)$, is formally generated by

$$P(q) = 1 + \sum_{n \geq 1} p(n) q^n = \prod_{n \geq 1} (1 - q^n)^{-1}. \tag{5.1.1}$$

One ignores "0" and permutations. Thus $p(5) = 7$ since

$$\begin{aligned} 5 &= 4+1 = 3+2 = 3+1+1 = 2+2+1 \\ &= 2+1+1+1 = 1+1+1+1+1. \end{aligned} \tag{5.1.2}$$

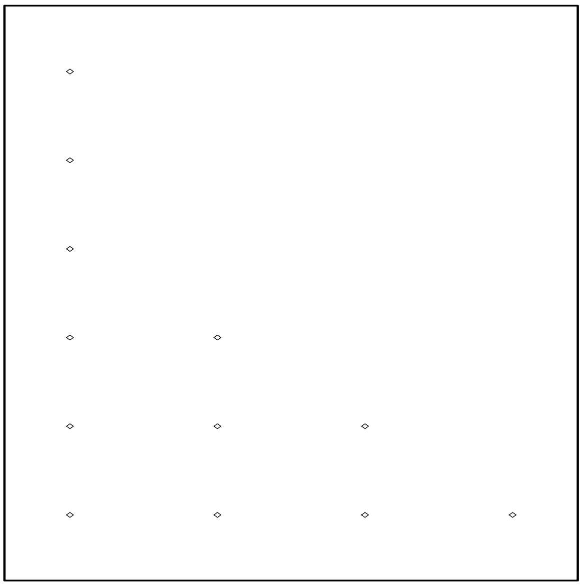

Figure 5.1: A Ferrer diagram

Additive partitions are less tractable than multiplicative ones as there is no analogue of unique prime factorization nor the corresponding structure.

Formula (5.1.1) is easily seen by expanding $(1-q^n)^{-1}$ and comparing coefficients. It is relatively easy to deduce that $2^{\sqrt{n}} < p(n) < e^{\pi\sqrt{2n/3}}$ for $n > 3$ (see [38]), and that the series is absolutely convergent for $|q| < 1$. We return to the analytic behavior of this series below.

Partitions provide a wonderful example of why Keith Devlin calls mathematics "the science of patterns" [26]. Many geometric representations exist. For example, the partition $5 = 4 + 1$ can be represented as a point at $(0, 0)$ and four points at $(0, 1), (1, 1), (2, 1), (3, 1)$. Read with axis reversed, this identifies $1 + 4$ with $2+1+1+1$ and so on. See Figure 5.1, which identifies $1+1+1+2+3+4$ and $6 + 3 + 2 + 1$. Such techniques provide alternate ways to prove results such as *the number of partitions of n with all parts odd is the number of partitions of n into distinct parts*, (see Volume 2, Chapter 4, Exercise 1).

A modern computational temperament leads to:

Question: How hard is $p(n)$ to compute—in 1900 (for MacMahon the "father of combinatorial analysis") or in 2000 (for *Maple* or *Mathematica*)?

Answer: The computation of $p(200) = 3972999029388$ took MacMahon months and intelligence. Now, however, we can use the most naive approach: Computing 200 terms of the series for the inverse product in (5.1.1) instantly produces the result using either *Mathematica* or *Maple*. Obtaining the result $p(500) = 2300165032574323995027$ is not much more difficult, using the *Maple* code

```
> N:=500; coeff(series(1/product(1-q^n,n=1..N+1),q,N+1),q,N);
```

$$2300165032574323995027$$

□

5.1.1 The "Exact" Formula for the Partition Function

[*From Volume 2, Section 4.1.3*]

One of the signal achievements of early twentieth century analysis was Hardy and Ramanujan's precise asymptotic for $p(n)$ [21]. It is based in part on an analysis of the *Dedekind η-function* $\eta(q) = e^{\pi iz/12}\prod_{n\geq 1}(1-e^{2\pi inz})$. The function η is closely related to $Q(q)$, and $\theta_3(q)$ discussed in the next section, and satisfies a modular equation. Their asymptotic is

$$p(n) = \frac{e^{K\lambda_n}}{4\sqrt{3}\lambda_n^2}\left(1+O\left(\frac{1}{\sqrt{n}}\right)\right), \tag{5.1.3}$$

where $K = \pi\sqrt{2/3}$ and $\lambda_n = \sqrt{n - 1/24}$.

This was subsequently refined by Rademacher to

$$p(n) = \frac{1}{\pi\sqrt{2}}\sum_{k=1}^{\infty}\alpha_k(n)\sqrt{k}\,\frac{d}{dx}\left[\frac{\sinh\left(\frac{\pi}{k}\sqrt{\frac{2}{3}\left(x-\frac{1}{24}\right)}\right)}{\sqrt{\left(x-\frac{1}{24}\right)}}\right]_{x=n}, \tag{5.1.4}$$

where

$$\alpha_k(n) = \sum_{(h,k)=1}^{k}\omega_{h,k}e^{-2\pi inh/k},$$

and $\omega_{h,k} = \exp(\pi i\tau_{h,k})$ with

$$\tau_{h,k} = \sum_{m=1}^{k-1}\left(\frac{m}{k}-\left\lfloor\frac{m}{k}\right\rfloor-\frac{1}{2}\right)\left(\frac{hm}{k}-\left\lfloor\frac{hm}{k}\right\rfloor-\frac{1}{2}\right).$$

If order $\sqrt{n}$ terms are appropriately used, the nearest integer is $p(n)$.

A mere five terms of this expansion provides $p(200) \approx 3972999029387.86108$ and six terms yields $p(500) \approx 2300165032574323995027.196661$. As we have seen, the underlying asymptotic is

$$p(n) \sim \frac{1}{4n\sqrt{3}}\, e^{\pi\sqrt{2n/3}}.$$

Later Erdős made an "elementary" derivation of the Hardy-Ramanujan formula (5.1.3). A recent discussion of this formula is given by Almkvist and Wilf in [2]. It is interesting to speculate how much corresponding beautiful mathematics is not done when computation becomes too easy—both *Maple* and *Mathematica* have good built-in partition functions.

5.2 Singular Values

[*From Volume 2, Section 4.2*]

The Jacobian theta functions are a very rich source mine for experimentation—both as a tool to learning classical theory and to discover new phenomena. Further details of what follows are given fully in [15]. For our purposes, we consider only the three classical θ-functions:

$$\begin{aligned} \theta_3(q) &= \sum_{n=-\infty}^{\infty} q^{n^2}, \qquad (5.2.5)\\ \theta_4(q) &= \sum_{n=-\infty}^{\infty} (-1)^n q^{n^2}, \\ \theta_2(q) &= \sum_{n=-\infty}^{\infty} q^{(n+1/2)^2}, \end{aligned}$$

for $|q| \le 1$. Note that θ_3^2 is the generating function for the number of ways of writing a number as a sum of two squares, counting order and sign. Similarly, θ_2^2 counts sums of two odd squares.

A beautiful result of Jacobi's is

$$\theta_3^4(q) = \theta_2^4(q) + \theta_4^4(q). \qquad (5.2.6)$$

If we write $k = \theta_2^2/\theta_3^2$ and $k' = \theta_4^2/\theta_3^2$, we note that $k^2 + (k')^2 = 1$. It transpires that

$$(i) \quad \theta_3^2(q^2) = \frac{\theta_4^2(q) + \theta_3^2(q)}{2} \qquad (ii) \quad \theta_4^2(q^2) = \theta_4(q)\,\theta_3(q). \tag{5.2.7}$$

Now (5.2.6) and (5.2.7) can be proved in many ways and can be "verified" symbolically in many more.

5.3 Some Fibonacci Sums

[*From Volume 2, Section 4.4*]

Theta functions turn up in quite unexpected places as we now show. The *Fibonacci sequence*, namely

$$1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, \cdots,$$

takes its name from its first appearance in print, which seems to have been in the famous book *Liber Abaci*, published by Leonardo Fibonacci (also known as Leonardo of Pisa) in 1202. He asked:

> How many pairs of rabbits can be produced from a single pair in a year if every month each pair begets a new pair which from the second month on becomes productive?

Lest one thinks the problem is imprecise, Fibonacci describes the solution in the text and in the margin. There one finds written vertically

> Parium 1 Primus 2 Secundus 3 Tercius 5 Quartus 8 Quintus 13 Sestus 21 Septimus 34 Octauus 55 Nonus 89 Decimus 144 Undecimus 233 Duodecimus 377.

We leave it to the reader to decide that this indeed leads to the Fibonacci sequence, but we do note that "the proof is left as an exercise" seems to have occurred first in *De Triangulis Omnimodis* by Regiomontanus, written in 1464 (but published in 1533). He is quoted as saying, "This is seen to be the converse of the preceding. Moreover, it has a straightforward proof, as did the preceding. Whereupon I leave it to you for homework."

Among its many other contributions such as popularizing Hindu-Arabic notation in the west, *Liber Abaci* contains methods for extracting cube roots, for solving quadratics, and the lovely identity $(a^2+b^2)(c^2+d^2) = (ac \pm bd)^2 + (ad \mp bc)^2$, which shows the product of sums of two squares is such a sum.

The Fibonacci sequence occurs in many contexts both serious and quirky. For example, 144 is the only Fibonacci square. A moment's inspection shows that it is generated by

$$F_0 = 1, \qquad F_1 = 1, \qquad F_{n+1} = F_n + F_{n-1}. \tag{5.3.8}$$

It grows quickly (like rabbits) and is monotonic. In particular, $F_{n+2} > 2\,F_n$. If we look computationally at F_{n+1}/F_n, for $n = 10, 20, 30, 40$, we obtain the numerical values $1.61818181818, 1.61803399852, 1.61803398875, 1.61803398875$, which either the human eye or a constant recognition facility reveals to be the *Golden Mean* $\phi = (\sqrt{5}+1)/2$, to the precision used.

Indeed, the standard theory of two term linear recurrence relations leads to

$$F_n = \frac{1}{\sqrt{5}} \left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n, \tag{5.3.9}$$

where $(1-\sqrt{5})/2$ is the other root of $x^2 = x + 1$.

It is easy to check that the sequence in (5.3.9) satisfies the recursion in (5.3.8), and has the correct initial conditions. Since $|g| < 1$, it is also easy to see that $F_{n+1}/F_n \to \phi$, as claimed, and to deduce many other identities such as $F_{n+1}\,F_{n-1} = F_n^2 + (-1)^n$ for $n \geq 2$.

There is a slightly less well known companion *Lucas sequence*, named after the French number theorist Edouard Lucas (1842–1891):

$$L_0 = 2, \qquad L_1 = 1, \qquad L_{n+1} = L_n + L_{n-1}, \tag{5.3.10}$$

which is correspondingly solved by

$$L_n = \left(\frac{\sqrt{5}+1}{2}\right)^n + \left(\frac{1-\sqrt{5}}{2}\right)^n. \tag{5.3.11}$$

As both Fibonacci and Lucas sequences are built of geometric sequences, it is clear that we can easily evaluate sums like $\sum_{n=1}^{N} F_n^k$, for positive integer k. What happens for negative integers is more interesting.

A preparatory lemma is useful ([15]):

Lemma 5.3.1 *For $0 < \beta < \alpha$ with $\alpha\beta = 1$,*

$$\sum_{n=1}^{\infty} \frac{1}{\alpha^n + \beta^n} = \sum_{n=1}^{\infty} \frac{\beta^n}{1+\beta^{2n}} = \theta_3^2(\beta), \tag{5.3.12}$$

$$\sum_{n=0}^{\infty} \frac{1}{\alpha^{2n+1} + \beta^{2n+1}} = \sum_{n=0}^{\infty} \frac{\beta^{2n+1}}{1+\beta^{2n+1}} = \frac{1}{4}\,\theta_2^2(\beta^2). \tag{5.3.13}$$

Proof. The proof of the first formula is a consequence of the result on theta functions in Volume 1, 4.3.1. This relies on confirming that

$$\sum_{n=1}^{\infty} \frac{\beta^n}{1+\beta^{2n}} = \sum_{n=0}^{\infty} (-1)^n \frac{\beta^{2n+1}}{1-\beta^{2n+1}}. \tag{5.3.14}$$

(Try expanding both sides as double sums.)

The second formula then follows by applying the first to α^2 and β^2, and then subtracting that result from the first to obtain $(\theta_3^2(\beta) - \theta_3^2(\beta^2))/4$, which equals $\theta_2^2(\beta^2)/4$. $\Box$

Two immediate consequences are

$$\sum_{n=0}^{\infty} \frac{1}{F_{2n+1}} = \frac{\sqrt{5}}{4}\,\theta_2^2\left(\frac{3-\sqrt{5}}{2}\right) \tag{5.3.15}$$

$$\sum_{n=1}^{\infty} \frac{1}{L_{2n}} = \frac{1}{4}\,\theta_3^2\left(\frac{3-\sqrt{5}}{2}\right) + \frac{1}{4}. \tag{5.3.16}$$

Two somewhat more elaborate derivations, (see [15], Section 3.7), lead to

$$\sum_{n=1}^{\infty} \frac{1}{F_n^2} = \frac{5}{24}\left(\theta_2^4\left(\frac{3-\sqrt{5}}{2}\right) - \theta_4^4\left(\frac{3-\sqrt{5}}{2}\right) + 1\right) \tag{5.3.17}$$

$$\sum_{n=1}^{\infty} \frac{1}{L_n^2} = \frac{1}{8}\left(\theta_3^4\left(\frac{3-\sqrt{5}}{2}\right) - 1\right). \tag{5.3.18}$$

Since it is known that the classical theta functions are transcendental for algebraic values $q, 0 < |q| < 1$, we discover the far-from-obvious result that the left-hand side of each of (5.3.15), (5.3.16), (5.3.18) is a transcendental number, as probably is (5.3.17).

Moreover, since both the initial sums and especially the theta functions are easy to compute numerically, we can hunt for other such identities using integer relation methods. In this way, we find:

$$\sum_{n=1}^{\infty} \frac{(-1)^n}{F_n^2} = \frac{5}{48}\left(2 - \theta_2^4\left(\frac{3-\sqrt{5}}{2}\right) - 2\,\theta_4^4\left(\frac{3-\sqrt{5}}{2}\right)\right), \quad (5.3.19)$$

and a host of more recondite identities.

By contrast, a remarkable elementary identity is

$$\sum_{n=0}^{\infty} \frac{1}{F_{2n+1}+F_{2k-1}} = \frac{(2k-1)\sqrt{5}}{2\,F_{2k-1}}, \quad (5.3.20)$$

for $k = 1, 2, 3, \cdots$. So while $\sum_{n=0}^{\infty} F_{2n+1}^{-1}$ is transcendental, $\sum_{n=0}^{\infty}(F_{2n+1}+1)^{-1} = \sqrt{5}/2$. If we compute the corresponding continued fractions of the two sums, we obtain the quite different results $[1, 1, 4, 1, 2, 3, 6, 2, 1, 3, 1, 189, 1, 3, 12]$ and $[1, 8, 2, 8, 2, 8, 2, 8, 2, 8]$ in partial confirmation.

5.4 Commentary and Additional Examples

[*From Volume 2, Chapter 4 Commentary*]

1. **A combinatorial determinant problem.** Find the determinant of

$$\begin{bmatrix} \binom{n}{p} & \binom{n}{p+1} & \binom{n}{p+2} \\ \binom{n+1}{p} & \binom{n+1}{p+1} & \binom{n+1}{p+2} \\ \binom{n+2}{p} & \binom{n+2}{p+1} & \binom{n+2}{p+2} \end{bmatrix}$$

$$\begin{bmatrix} \binom{n}{p} & \binom{n}{p+1} & \binom{n}{p+2} & \binom{n}{p+3} \\ \binom{n+1}{p} & \binom{n+1}{p+1} & \binom{n+1}{p+2} & \binom{n+1}{p+3} \\ \binom{n+2}{p} & \binom{n+2}{p+1} & \binom{n+2}{p+2} & \binom{n+2}{p+3} \\ \binom{n+3}{p} & \binom{n+3}{p+1} & \binom{n+3}{p+2} & \binom{n+3}{p+3} \end{bmatrix}$$

and its q-dimensional extension as a function of n, p, q. (Taken from [32].)

Solution: The pattern is clear from the first few cases on simplifying in *Maple* or *Mathematica*.

2. **A sum-of-powers determinant.** Find the determinant of

$$\begin{bmatrix} \sum_{k=0}^{1} k^4 & \sum_{k=0}^{1} k^4 & \sum_{k=0}^{1} k^4 & \sum_{k=0}^{1} k^4 \\ \sum_{k=0}^{1} k^4 & \sum_{k=0}^{2} k^4 & \sum_{k=0}^{2} k^4 & \sum_{k=0}^{2} k^4 \\ \sum_{k=0}^{1} k^4 & \sum_{k=0}^{2} k^4 & \sum_{k=0}^{3} k^4 & \sum_{k=0}^{3} k^4 \\ \sum_{k=0}^{1} k^4 & \sum_{k=0}^{2} k^4 & \sum_{k=0}^{3} k^4 & \sum_{k=0}^{4} k^4 \end{bmatrix}$$

and its q-dimensional extension. (Taken from [32].)

Solution: The first few instances of this sequence are

$$1, 4, 216, 331776, 24883200000, 139314069504000000,$$

which can be quickly identified as $(q!)^q$, using the Sloane online sequence recognition tool. This fact can be proved by taking cofactors on the last row, and observing that only the final two entries have nonzero cofactors with value $(q-1)!^{q-1}$.

3. **Putnam problem 1994–B4.** Let d_n be the greatest common divisor of the entries of $A^n - I$ where $A = \begin{bmatrix} 3 & 2 \\ 4 & 3 \end{bmatrix}$. Show that $d_n \to \infty$ with n. Hint: Observe numerically, then prove by induction, that A^n has determinant 1 and is of the form $\begin{bmatrix} a_n & b_n \\ 2b_n & a_n \end{bmatrix}$. Hence, $(a_n - 1)|2b_n^2$. Then write A^n explicitly via the Cayley-Hamilton theorem, which tells us that $A^{n+1} = 6\,A^n - A^{n-1}$.

4. **Crandall's integral representation for Madelung's constant.** The following identity is both beautiful and effective—though less effective for computational purposes than Benson's formula. For example, 60 digits of $\mathcal{M}_3(1)$ can be obtained in seconds in *Maple* or *Mathematica* using Benson's identity, while using the numerical quadrature tools of Section 6.1 (see also

Volume 2, Section 7.4) to compute the integral to the same 60 digits takes roughly one hour runtime on a 2003-era computer. Richard Crandall's formula is derived in [23] from the Andrews formula for θ_2^3. It is

$$\begin{aligned}\mathcal{M}_3(1) &= -\frac{2}{\pi}\int_0^1 r\,dr\int_{-\pi}^{\pi}\frac{1+2/(1+r^{2(1-\sin\theta)})}{(1+r^{1+\cos\theta})(1+r^{1-\cos\theta})}\,d\theta \\ &= -1.7475645946332\ldots \qquad (5.4.21)\end{aligned}$$

5. **A polygon problem.** Count (i) the number of ways a polygon with $n+2$ sides can be cut into n triangles; (ii) the number of ways in which parentheses can be placed in a sequence of numbers to be multiplied, two at a time; and (iii) the number of paths of length $2n$ through an n-by-n grid that do not rise above the main diagonal (*Dijk paths*).

   Hint: In each case the sequence starts

$$1, 2, 5, 14, 42, 132, 429, 1430, 4862.$$

   The "gfun" package returns the generating function $4\left(1+\sqrt{1-4x}\right)^{-2}$ and the recursion $(4n+6)u(n) = (n+3)u(n+1)$, which gives rise to the Catalan numbers $(1/(n+1))\binom{2n}{n}$ named after Eugéne Charles Catalan (1814–1894).

6. **Fibonacci and Lucas numbers in terms of hyperbolic functions.** Show that

$$F_n = \frac{2}{\sqrt{5}}\, i^{-n}\sinh(n\theta) \qquad \text{and} \qquad L_n = 2\, i^{-n}\cosh(n\theta),$$

   where

$$\theta = \log\left(\frac{\sqrt{5}+1}{2}\right) + i\,\frac{\pi}{2}.$$

   Many Fibonacci formulas are then easy to obtain from the addition formulas for sinh and cosh—for example consider $5\,F_n^2 - L_n^2$. (See [27], which should be consulted whenever one "discovers" a result in classical number theory.)

Chapter 6

Numerical Techniques II

> Another thing I must point out is that you cannot prove a vague theory wrong . . . Also, if the process of computing the consequences is indefinite, then with a little skill any experimental result can be made to look like the expected consequences.
>
> Richard Feynman, 1964, from Gary Taubes, *The (Political) Science of Salt*, 1998

In this chapter, we will examine in more detail some additional underlying computational techniques that are useful in experimental mathematics. In particular, we shall briefly examine techniques for theorem proving, prime number computations, polynomial root finding, numerical quadrature, and infinte series summation. As in the first volume, 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.

6.1 Numerical Quadrature

[*From Volume 2, Section 7.4*]

Experimental mathematicians very frequently find it necessary to calculate definite integrals to high precision. Recall the examples given in Chapters 1 and 5 of the first volume, wherein we were able to experimentally identify certain definite integrals as analytic expressions, based only on their high-precision numerical value.

To briefly reprise one example, we were inspired by a recent problem in the *American Mathematical Monthly* [1]. By using one of the quadrature routines to be described below, together with a PSLQ integer relation detection program, we found that if $C(a)$ is defined by

$$C(a) = \int_0^1 \frac{\arctan(\sqrt{x^2+a^2})\,dx}{\sqrt{x^2+a^2}(x^2+1)}, \tag{6.1.1}$$

then

$$\begin{aligned} C(0) &= \pi \log 2/8 + G/2 \\ C(1) &= \pi/4 - \pi\sqrt{2}/2 + 3\sqrt{2}\arctan(\sqrt{2})/2 \\ C(\sqrt{2}) &= 5\pi^2/96, \end{aligned} \tag{6.1.2}$$

where $G = \sum_{k\geq 0}(-1)^k/(2k+1)^2$ is Catalan's constant. The third of these results is the result from the *Monthly*. These particular results then led to the following general result, among others:

$$\int_0^\infty \frac{\arctan(\sqrt{x^2+a^2})\,dx}{\sqrt{x^2+a^2}(x^2+1)} = \frac{\pi}{2\sqrt{a^2-1}}\left[2\arctan(\sqrt{a^2-1}) - \arctan(\sqrt{a^4-1})\right]. \tag{6.1.3}$$

The commercial packages *Maple* and *Mathematica* both include rather good high-precision numerical quadrature facilities. However, these packages do have some limitations, and in many cases much faster performance can be achieved with custom-written programs. And in general it is beneficial to have some understanding of quadrature techniques, even if you rely on software packages to perform the actual computation.

We describe here three state-of-the-art, highly efficient techniques for numerical quadrature. You can try programming these schemes yourself, or you can refer to the C++ and Fortran-90 programs available at http://www.expmath.info.

6.1.1 Error Function Quadrature

[*From Volume 2, Section 7.4.2*]

The second scheme we will discuss here is known as "error function" or "erf" quadrature. While error function quadrature is not as efficient as Gaussian quadrature for continuous, bounded, well-behaved functions on finite intervals, it often produces highly accurate results even for functions with (integrable) singularities or vertical derivatives at one or both endpoints of the interval. In contrast, Gaussian quadrature typically performs very poorly in such instances.

The error function quadrature scheme and the tanh-sinh scheme to be described in the next section are based on the Euler-Maclaurin summation formula, which can be stated as follows [4, pg. 280]. Let $m \geq 0$ and $n \geq 1$ be integers, and define $h = (b-a)/n$ and $x_j = a + jh$ for $0 \leq j \leq n$. Further, assume that the function $f(x)$ is at least $(2m+2)$-times continuously differentiable on $[a, b]$. Then

$$\begin{aligned} \int_a^b f(x)\,dx &= h \sum_{j=0}^{n} f(x_j) - \frac{h}{2}\left(f(a) + f(b)\right) \\ &\quad - \sum_{i=1}^{m} \frac{h^{2i} B_{2i}}{(2i)!}\left(f^{(2i-1)}(b) - f^{(2i-1)}(a)\right) - E, \end{aligned} \tag{6.1.4}$$

where B_{2i} denote the Bernoulli numbers, and

$$E = \frac{h^{2m+2}(b-a)B_{2m+2}f^{(2m+2)}(\xi)}{(2m+2)!}, \tag{6.1.5}$$

for some $\xi \in (a, b)$.

In the circumstance where the function $f(x)$ and all of its derivatives are zero at the endpoints a and b, the second and third terms of the Euler-Maclaurin formula are zero. Thus the error in a simple step-function approximation to the integral, with interval h, is simply E. But since E is then less than a constant times $h^{2m+2}/(2m+2)!$, for any m, we conclude that the error goes to zero more rapidly than any power of h. In the case of a function defined on $(-\infty, \infty)$, the Euler-Maclaurin summation formula still applies to the resulting doubly infinite sum approximation, provided as before that the function and all of its derivatives tend to zero for large positive and negative arguments.

This principle is utilized in the error function and tanh-sinh quadrature scheme by transforming the integral of $f(x)$ on a finite interval, which we will take to be $(-1, 1)$ for convenience, to an integral on $(-\infty, \infty)$ using the change of variable $x = g(t)$. Here $g(x)$ is some monotonic function with the property that

$g(x) \to 1$ as $x \to \infty$, and $g(x) \to -1$ as $x \to -\infty$, and also with the property that $g'(x)$ and all higher derivatives rapidly approach zero for large arguments. In this case we can write, for $h > 0$,

$$\int_{-1}^{1} f(x)\,dx \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\,dt \;=\; h\sum_{-\infty}^{\infty} w_j f(x_j), \tag{6.1.6}$$

where $x_j = g(hj)$ and $w_j = g'(hj)$. If the convergence of $g'(t)$ and its derivatives to zero is sufficiently rapid for large $|t|$, then even in cases where $f(x)$ has a vertical derivative or an integrable singularity at one or both endpoints, the resulting integrand $f(g(t))g'(t)$ will be a smooth bell-shaped function for which the Euler-Maclaurin summation formula applies, as described above. In such cases we have that the error in the above approximation decreases faster than any power of h. The summation above is typically carried out to limits $(-N, N)$, beyond which the terms of the summand are less than the "epsilon" of the multiprecision arithmetic being used.

The error function integration scheme uses the function $g(t) = \mathrm{erf}(t)$ and $g'(t) = (2/\sqrt{\pi})e^{-t^2}$. Note that $g'(t)$ is merely the bell-shaped probability density function, which is well known to converge rapidly to zero, together with all of its derivatives, for large arguments. The error function $\mathrm{erf}(x)$ can be computed to high precision as $1 - \mathrm{erfc}(x)$, using the following formula given by Crandall [22, pg. 85] (who in turn attributes it to a 1968 paper by Chiarella and Reichel):

$$\mathrm{erfc}(t) \;=\; \frac{e^{-t^2}\alpha t}{\pi}\left(\frac{1}{t^2} + 2\sum_{k\ge 1}\frac{e^{-k^2\alpha^2}}{k^2\alpha^2 + t^2}\right) + \frac{2}{1 - e^{2\pi t/\alpha}} + E, \tag{6.1.7}$$

where $|E| < e^{-\pi^2/\alpha^2}$. The parameter $\alpha > 0$ here is chosen small enough to ensure that the error E is sufficiently small. We summarize this scheme with the following algorithm statement. Here n_p is the precision level in digits, and ϵ is the "epsilon" level, which is typically 10^{-n_p}.

Algorithm 4 *Error function complement [erfc] evaluation.*

Initialize:
Set $\alpha := \pi/\sqrt{n_p \log(10)}$, and set $n_t := n_p \log(10)/\pi$.
Set $t_2 := e^{-\alpha^2}$, $t_3 := t_2^2$, and $t_4 := 1$.

For $k := 1$ to n_t do: set $t_4 := t_2 \cdot t_4,\ E_k := t_4,\ t_2 := t_2 \cdot t_3$; enddo.

Evaluation of function, with argument x:
Set $t_1 := 0,\ t_2 := x^2,\ t_3 := e^{-t_2}$ and $t_4 := \epsilon/(1000 \cdot t_3)$.
For $k := 1$ to n_t do: set $t_5 := E_k/(k^2\alpha^2 + t_2)$ and $t_1 := t_1 + t_5$.
If $|t_5| < t_4$ then exit do; enddo.
Set $\text{erfc}(x) := t_3\alpha x/\pi \cdot (1/t_2 + 2t_1) + 2/(1 - e^{2\pi x/\alpha})$. □

We now state the algorithm for error function quadrature. As with the Gaussian scheme, m levels or phases of abscissas and weights are precomputed in the error function scheme. Then we perform the computation, increasing the level by one (each of which approximately doubles the computation, compared to the previous level), until an acceptable level of estimated accuracy is obtained (see Volume 2, Section 7.4.4 for an efficient error estimation). In the following, ϵ is the "epsilon" level of the multiprecision arithmetic being used.

Algorithm 5 *Error function quadrature.*

Initialize:
Set $h := 2^{2-m}$.
For $k := 0$ to $20 \cdot 2^m$ do:
Set $t := kh,\ x_k := 1 - \text{erfc}(t)$ and $w_k := 2/\sqrt{\pi} \cdot e^{-t^2}$.
If $|x_k - 1| < \epsilon$ then exit do; enddo.
Set $n_t = k$ (the value of k at exit).

Perform quadrature for a function $f(x)$ on $(-1, 1)$:
Set $S := 0$ and $h := 4$.
For $k := 1$ to m (or until successive values of S are identical to within ϵ) do:
$h := h/2$.
For $i := 0$ to n_t step 2^{m-k} do:
If $(\text{mod}(i, 2^{m-k+1}) \neq 0$ or $k = 1)$ then
If $i = 0$ then $S := S + w_0 f(0)$ else $S := S + w_i(f(-x_i) + f(x_i))$ endif.
endif; enddo; endo.
Result $= hS$. □

6.2 Commentary and Additional Examples

[*From Volume 2, Chapter 7 Commentary*]

1. **Evaluation of integrals.** Evaluate the following integrals, by numerically computing them and then trying to recognize the answers, either by using the Inverse Symbolic Calculator at http://www.cecm.sfu.ca/projects/ISC, or by using a PSLQ facility, such as that built into the Experimental Mathematician's Toolkit, available at http://www.expmath.info.

   These examples are taken from Gradsteyn and Ryzhik [31]. All of the answers are simple one- or few-term expressions involving familiar mathematical constants such as π, e, $\sqrt{2}$, $\sqrt{3}$, $\log 2$, $\zeta(3)$, G (Catalan's constant), and γ (Euler's constant). We recognize that many of these can be evaluated analytically using symbolic computing software (depending on the available versions). The intent here is to provide exercises for numerical quadrature and constant recognition facilities.

$$\text{(a)} \qquad \int_0^1 \frac{x^2\,dx}{(1+x^4)\sqrt{1-x^4}} \tag{6.2.8}$$

$$\text{(b)} \qquad \int_0^\infty x e^{-x}\sqrt{1-e^{-2x}}\,dx \tag{6.2.9}$$

$$\text{(c)} \qquad \int_0^\infty \frac{x^2\,dx}{\sqrt{e^x-1}} \tag{6.2.10}$$

$$\text{(d)} \qquad \int_0^{\pi/4} x\tan x\,dx \tag{6.2.11}$$

$$\text{(e)} \qquad \int_0^{\pi/2} \frac{x^2\,dx}{1-\cos x} \tag{6.2.12}$$

$$\text{(f)} \qquad \int_0^{\pi/4} (\pi/4 - x\tan x)\tan x\,dx \tag{6.2.13}$$

$$\text{(g)} \qquad \int_0^{\pi/2} \log^2(\cos x)\,dx \tag{6.2.14}$$

   Answers: (a) $\pi/8$, (b) $\pi(1+2\log 2)/8$, (c) $4\pi(\log^2 2+\pi^2/12)$, (d) $(\pi\log 2)/8+G/2$, (e) $-\pi^2/4+\pi\log 2+4G$, (f) $(\log 2)/2+\pi^2/32-\pi/4+(\pi\log 2)/8$, (g) $\pi/2(\log^2 2+\pi^2/12)$.

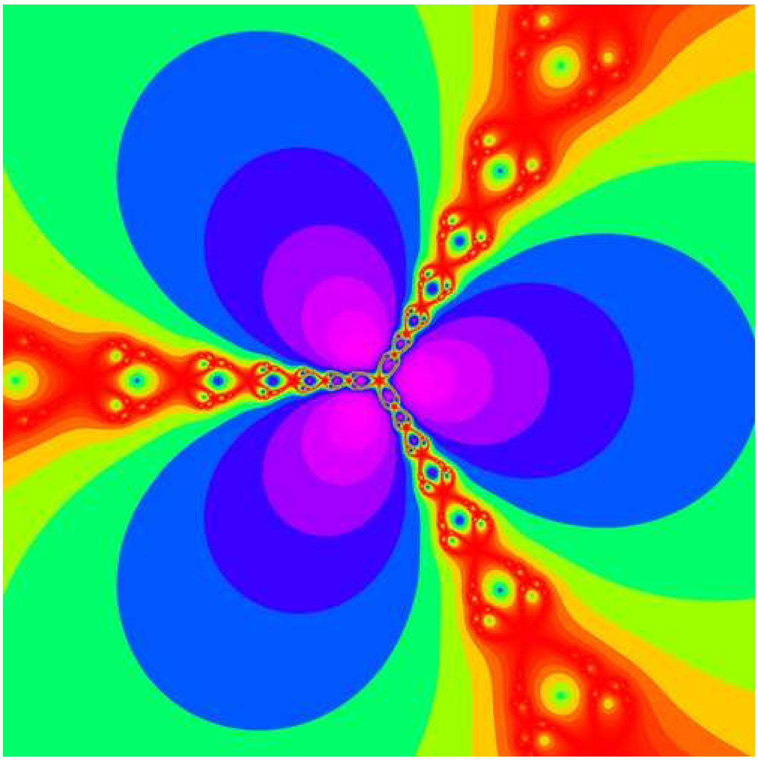

Figure 6.1: Newton-Julia set for $p(x) = x^3 - 1$.

2. **Julia sets.** Figure 6.1 is a color-coded plot of the number of iterations required for convergence (to some accuracy ϵ) of Newton's iteration (in the complex plane) for the cubic polynomial $p(x) = x^3 - 1$. The filamentary structure shown is a *Julia set*, a set of measure zero separating disconnected regions.

3. **Chaitin on randomness.** It seems apropos to end with Greg Chaitin's views in "The Creative Life: Science vs Art," an article available at the URL http://www.cs.umaine.edu/~chaitin/cdg.html.

> The message is that mathematics is quasi-empirical, that mathematics is not the same as physics, not an empirical science, but I think it's more akin to an empirical science than mathematicians would like to admit.

Mathematicians normally think that they possess absolute truth. They read God's thoughts. They have absolute certainty and all the rest of us have doubts. Even the best physics is uncertain, it is tentative. Newtonian science was replaced by relativity theory, and then—wrong!—quantum mechanics showed that relativity theory is incorrect. But mathematicians like to think that mathematics is forever, that it is eternal. Well, there is an element of that. Certainly a mathematical proof gives more certainty than an argument in physics or than experimental evidence, but mathematics is not certain. This is the real message of Gödel's famous incompleteness theorem and of Turing's work on uncomputability.

You see, with Gödel and Turing the notion that mathematics has limitations seems very shocking and surprising. But my theory just measures mathematical information. Once you measure mathematical information you see that any mathematical theory can only have a finite amount of information. But the world of mathematics has an infinite amount of information. Therefore it is natural that any given mathematical theory is limited, the same way that as physics progresses you need new laws of physics. Mathematicians like to think that they know all the laws. My work suggests that mathematicians also have to add new axioms, simply because there is an infinite amount of mathematical information. This is very controversial. I think mathematicians, in general, hate my ideas. Physicists love my ideas because I am saying that mathematics has some of the uncertainties and some of the characteristics of physics. Another aspect of my work is that I found randomness in the foundations of mathematics. Mathematicians either don't understand that assertion or else it is a nightmare for them ...

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[2]In this Index, † denotes a quote.