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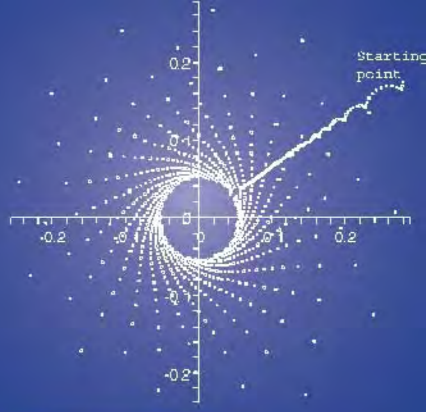
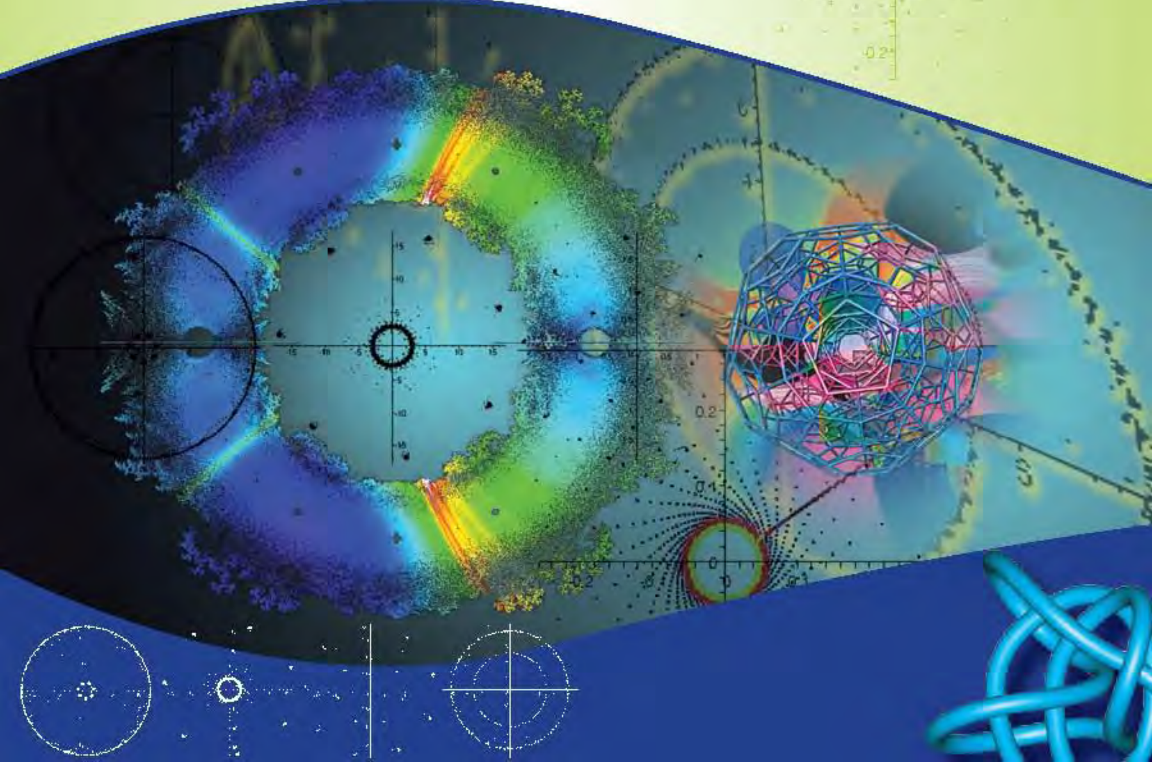


Experimental Mathematics in Action



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To our spouses, children, grandchildren, students, and all lovers of
experimental mathematics

Contents

Preface

This book originated with a short course of the same name, sponsored by the Mathematical Association of America (MAA) at its annual meeting in San Antonio, January 2006. The abstract for our course began:

> This two-day Short Course on Experimental Mathematics in Action is organized by Jonathan M. Borwein, Dalhousie University, and will take place on Tuesday and Wednesday, January 10 and 11. While a working knowledge of some mathematical computing package is an advantage, it is certainly not a prerequisite. Additionally, the course will be "hands on" for those who wish to follow along using their laptops, via a wireless Internet connection.
>
> The last twenty years have been witness to a fundamental shift in the way mathematics is practiced. With the continued advance of computing power and accessibility, the view that "real mathematicians don't compute" no longer has any traction for a newer generation of mathematicians that can really take advantage of computer aided research, especially given the modern computational packages such as *Maple*, *Mathematica*, and *Matlab*.
>
> The goal of this course is to present a coherent variety of accessible examples of modern mathematics where intelligent computing plays a significant role and in doing so to highlight some of the key algorithms and to teach some of the key experimental approaches.

The course consisted of eight lectures over two days—one for each of the eight main chapters of the book, given in order except that Chapter 3 was moved to the penultimate spot. A full draft version of the book was prepared before the short course was given and was subsequently revised and polished in light of experience gained. A complete record of the course is preserved at http://www.experimentalmath.info/maa-course.

Two of the authors, Bailey and Borwein, had already established a website containing an updated collection of links to many of the URLs mentioned in their two earlier volumes, plus errata, software, tools, and other useful information on experimental mathematics. This can be found at [15] http://www.experimentalmath.info.

The authors would like to thank the Mathematical Association of America (MAA) for the opportunity to develop this course. We are very grateful to A K Peters for enthusiastically agreeing to publish the corresponding book and for all the assistance offered by Charlotte Henderson and others at A K Peters. Also, we should like to thank all of our colleagues who have shared their experimental mathematics experiences with us. We especially wish to thank Eva Curry and Chris Hamilton who assisted in many ways with both content and technical matters.

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1 A Philosophical Introduction

> Whether we scientists are inspired, bored, or infuriated by philosophy, all our theorizing and experimentation depends on particular philosophical background assumptions. This hidden influence is an acute embarrassment to many researchers, and it is therefore not often acknowledged.
>
> —Christopher Koch [182]

1.1 Introduction

Christopher Koch, in the quote above, accurately captures a great scientific distaste for philosophizing. That acknowledged, we are of the opinion that mathematical philosophy matters more now than it has in nearly a century. The power of modern computers matched with that of modern mathematical software and the sophistication of current mathematics is changing the way we do mathematics.

In our view it is now both necessary and possible to admit quasi-empirical inductive methods fully into mathematical argument. In doing so carefully we will enrich mathematics and yet preserve the mathematical literature's deserved reputation for reliability—even as the methods and criteria change.

1.2 Mathematical Knowledge as We View It

Somewhat unusually, one of the authors (Jonathan Borwein) can exactly place the day at registration that he became a mathematician and recalls the reason why. "I was about to deposit my punch cards in the honours history bin. I remember thinking

> If I do study history, in ten years I shall have forgotten how to use the calculus properly. If I take mathematics, I shall still be able to read competently about the War of 1812 or the Papal schism. (Jonathan Borwein, 1968)

"The inescapable reality of objective mathematical knowledge is still with me. Nonetheless, my view then of the edifice I was entering is not that close to my view of the one I inhabit nearly forty years later.

"I also know when I became a computer-assisted fallibilist. Reading Imre Lakatos' *Proofs and Refutations* [189] a few years later while a very new faculty member, I was suddenly absolved from the grave sin of error, as I began to understand that missteps, mistakes and errors are the grist of all creative work. The book, his doctorate posthumously published in 1976, is a student conversation about the Euler characteristic. The students are of various philosophical stripes and the discourse benefits from his early work on Hegel with the Stalinist Lukács in Hungary and from later study with Karl Popper at the London School of Economics. I had been prepared for this dispensation by the opportunity to learn a variety of subjects from Michael Dummett. Dummett was at that time completing his study rehabilitating Frege's status [122].

"A decade later the appearance of the first 'portable' computers happily coincided with my desire to decode Srinivasa Ramanujan's (1887–1920) cryptic assertions about theta functions and elliptic integrals [53]. I realized that by coding his formulae and my own in the APL programming language,[1] I was able to rapidly confirm and refute identities and conjectures and to travel much more rapidly and fearlessly down potential blind alleys. I had become a computer-assisted fallibilist; at first somewhat falteringly but twenty years have certainly honed my abilities.

"Today, while I appreciate fine proofs and aim to produce them when possible, I no longer view proof as the royal road to secure mathematical knowledge."

1.3 Mathematical Reasoning

We first discuss our views, and those of others, on the nature of mathematics, and then illustrate these views in a variety of mathematical contexts. A considerably more detailed treatment of many of these topics is to be found in the book, by two of the current authors (D. Bailey and J. Borwein), *Mathematics by Experiment: Plausible Reasoning in the 21st Century*—especially in Chapters One, Two, and Seven.

Kurt Gödel may well have overturned the mathematical apple cart entirely deductively, but nonetheless he could hold quite different ideas about legitimate forms of mathematical reasoning [146]:

> 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,[2] 1951)

[1] Known as a 'write only,' very high level language, APL was a fine tool—albeit with a steep learning curve—whose code is almost impossible to read later.

[2] Taken from a previously unpublished work [146].

While we mathematicians have often separated ourselves from the sciences, they have tended to be more ecumenical. For example, a recent review of *Models: The Third Dimension of Science* [78] chose a mathematical plaster model of a Clebsch diagonal surface as its only illustration. Similarly, authors seeking examples of the aesthetic in science often choose iconic mathematics formulas such as $E = mc^2$.

Let us begin by fixing a few concepts before starting work in earnest. Above all, we hope to persuade you of the great power of mathematical experimentation—it is also fun—and that the traditional accounting of mathematical learning and research is largely an ahistorical caricature. We recall three terms.

> *mathematics, n.* a group of related subjects, including algebra, geometry, trigonometry, and calculus, concerned with the study of number, quantity, shape, and space and their inter-relationships, applications, generalizations, and abstractions.

This definition—taken from the Collins Dictionary [46]—makes no immediate mention of proof, nor of the means of reasoning to be allowed. The Webster's Dictionary [245] contrasts

> *induction, n.* any form of reasoning in which the conclusion, though supported by the premises, does not follow from them necessarily;

and

> *deduction, n.* a. a process of reasoning in which a conclusion follows necessarily from the premises presented, so that the conclusion cannot be false if the premises are true. b. a conclusion reached by this process.

Like Gödel, we suggest that both should be entertained in mathematics. This is certainly compatible with the general view of mathematicians that in some sense "mathematical stuff is out there" to be discovered. In this book, we shall talk broadly about experimental and heuristic mathematics, giving accessible, primarily visual and symbolic, examples.

1.4 Philosophy of Experimental Mathematics

> Our central mission is to compute quantities that are typically uncomputable, from an analytical point of view, and to do it with lightning speed.
>
> —Nick Trefethen [266]

The shift from *typographic* to *digital culture* is vexing for mathematicians. For example, there is still no truly satisfactory way of displaying mathematics on the web—and certainly not of asking mathematical questions. Also, we respect *authority* [148] but value *authorship* deeply—however much the two values are in conflict [69]. For example, the more we recast someone else's ideas in our own words, the more we enhance our authorship while undermining the original authority of the notions. Medieval scribes had the opposite concern and so took care to attribute their ideas to such as Aristotle or Plato.

And mathematicians care more about the *reliability* of our literature than does any other science. Indeed, one could argue that we have reified this notion and often pay lip-service, not real attention, to our older literature. How often does one see original sources sprinkled like holy water in papers that make no real use of them?

The traditional central role of proof in mathematics is arguably and perhaps appropriately under siege. Via examples, we intend to pose and answer various questions. We shall conclude with a variety of quotations from our progenitors and even contemporaries.

Our Questions. What constitutes secure mathematical knowledge? When is computation convincing? Are humans less fallible? What tools are available? What methodologies? What of the "law of the small numbers"? Who cares for certainty? What is the role of proof? How is mathematics actually done? How should it be? We mean these questions both about the apprehension (discovery) and the establishment (proving) of mathematics. This is presumably more controversial in the formal proof phase.

Our Answers. To misquote D'Arcy Thompson (1860–1948) "form follows function" [263]: rigour (proof) follows reason (discovery); indeed, excessive focus on rigour has driven us away from our wellsprings. Many good ideas are wrong. Not all truths are provable, and not all provable truths are worth proving .... Gödel's incompleteness results certainly showed us the first two of these assertions while the third is the bane of editors who are frequently presented with correct but unexceptional and unmotivated generalizations of results in the literature. Moreover, near certainty is often as good as it gets—intellectual context (community) matters. Recent complex human proofs are often very long, extraordinarily subtle and fraught with error—consider Fermat's last theorem, the Poincaré conjecture, the classification of finite simple groups, presumably any proof of the *Riemann hypothesis* (RH)[3] [241]. So while we mathematicians publicly talk of certainty, we really settle for security.

In all these settings, modern computational tools dramatically change the nature and scale of available evidence. Given an interesting identity buried in a long and complicated paper on an unfamiliar subject, which would give you more con-

[3] All nontrivial zeroes—nonnegative even integers—of the zeta function lie on the line with real part 1/2.

fidence in its correctness: staring at the proof, or confirming computationally that it is correct to 10,000 decimal places?

Here is such a formula [13]:

$$\frac{24}{7\sqrt{7}}\int_{\pi/3}^{\pi/2}\log\left|\frac{\tan t+\sqrt{7}}{\tan t-\sqrt{7}}\right|dt \stackrel{?}{=} L_{-7}(2) \tag{1.1}$$
$$= \sum_{n=0}^{\infty}\left[\frac{1}{(7n+1)^2}+\frac{1}{(7n+2)^2}-\frac{1}{(7n+3)^2}+\frac{1}{(7n+4)^2}-\frac{1}{(7n+5)^2}-\frac{1}{(7n+6)^2}\right].$$

This identity links a volume (the integral) to an arithmetic quantity (the sum). It arose out of some studies in quantum field theory, in analysis of the volumes of ideal tetrahedra in hyperbolic space. The question mark is used because, while no hint of a path to a formal proof is yet known, it has been verified numerically to 20,000 digit precision—using 45 minutes on 1024 processors at Virginia Tech.

A more inductive approach can have significant benefits. For example, as there is still some doubt about the proof of the classification of finite simple groups, it is important to ask whether the result is true but the proof flawed, or rather if there is still perhaps an "ogre" sporadic group even larger than the "monster"? What heuristic, probabilistic or computational tools can increase our confidence that the ogre does or does not exist? Likewise, there are experts who still believe that (RH) may be false and that the billions of zeroes found so far are much too small to be representative.[4] In any event, our understanding of the complexity of various crypto-systems relies on (RH) and we should like secure knowledge that any counterexample is enormous.

Peter Medawar (1915–1987). Medawar, a Nobel prize winning oncologist and a great expositor of science, writing in *Advice to a Young Scientist* [212] identifies four forms of scientific experiment:

1. *The Kantian experiment generates "the classical non-Euclidean geometries (hyperbolic, elliptic) by replacing Euclid's axiom of parallels (or something equivalent to it) with alternative forms."* All mathematicians perform such experiments while the majority of computer explorations are of the following Baconian form.

2. *The Baconian experiment is a contrived as opposed to a natural happening, it "is the consequence of 'trying things out' or even of merely messing*

[4]See [224] and various of Andrew Odlyzko's unpublished but widely circulated works.

about." Baconian experiments are the explorations of a happy if disorganized beachcomber and carry little predictive power.

3. *Aristotelian demonstrations "apply electrodes to a frog's sciatic nerve, and lo, the leg kicks; always precede the presentation of the dog's dinner with the ringing of a bell, and lo, the bell alone will soon make the dog dribble."* Arguably our "Corollaries" and "Examples" are Aristotelian, they reinforce but do not predict. Medawar then says the most important form of experiment is:

4. *The Galilean experiment is "a critical experiment—one that discriminates between possibilities and, in doing so, either gives us confidence in the view we are taking or makes us think it in need of correction."* The Galilean is the only form of experiment which stands to make experimental mathematics a serious enterprise. Performing careful, replicable Galilean experiments requires work and care.

Figure 1.1 illustrates the roles of the different kinds of experiments in the process of science. This model of the "science process" was created by Thomas Daske and Manuel Tomas, two students who took part in a seminar about *Experimental Mathematics in Action* and had the task to prepare a presentation about this chapter.

Their model assumes *science* to be any process that creates knowledge: more precisely empirical, as opposed to belief-based or revealed, knowledge. Formalism is a way to organize knowledge, to increase certainty—of special importance of course in mathematics. New knowledge is then obtained mainly through a combination of observation and experimentation.

The most primitive form of this is pure observation, without much aim or structure. If there is any experimentation going on at this stage, it will be mostly *Baconian*. Sometimes, if enough observations are accumulated, they can become a "critical mass": patterns and structures may become visible which can then be explored—by *Aristotelian* experimentation, trying to reproduce effects. The results of this experimentation may then serve to solidify intuition into something more tangible. In mathematics, at least, this step is often already followed by formalization, and formalization in turn is always accompanied by a testing of hypotheses and assumptions, in other words by *Kantian* experiments. In this stage, often *Galilean* experimentation also already begins: Can this property be extended to a larger class of objects? Indeed, the ruling out of counterexamples in some subclass is certainly a result which discriminates between possibilities and enhances confidence, while not providing absolute certainty. And after the formalism is fixed and the assumptions are clear, there is more *Galilean* experimen-

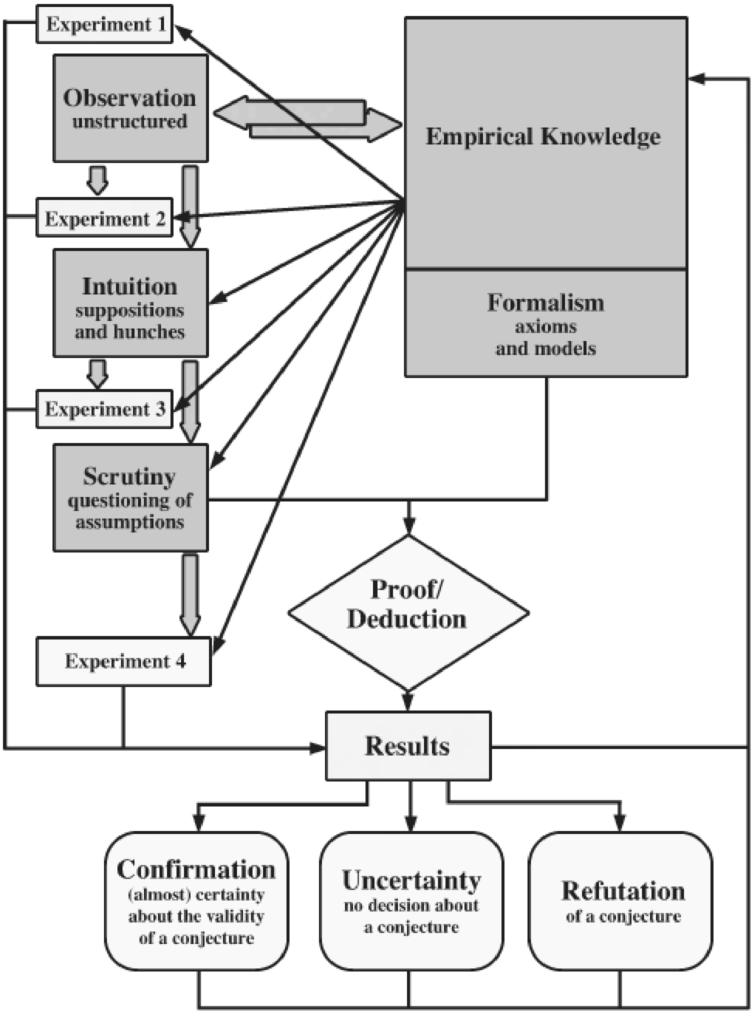


Figure 1.1. Modelling the role of experiments in the scientific process (T. Daske & M. Tomas).

tation; replicable, well-designed, discriminating experiments in the framework of the respective theory.

This process is less straightforward than it is iterative; in each step the results of the experiments may directly change the knowledge base, which then in turn may set into motion other steps in the scientific process.

Reuben Hersh (1927–). Hersh's arguments for a humanist philosophy of mathematics [165, 166], as paraphrased below, become even more convincing in our highly computational setting.

1. *Mathematics is human.* It is part of and fits into human culture. It does not match Frege's concept of an abstract, timeless, tenseless, objective reality.[5]

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

3. *There are different versions of proof or rigor.* Standards of rigor can vary depending on time, place, and other things. The use of computers in formal proofs, exemplified by the computer-assisted proof of the four color theorem in 1977,[6] is just one example of an emerging nontraditional standard of rigor.

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

5. *Mathematical objects are a special variety of a social-cultural-historical object.* Contrary to the assertions of certain postmodern detractors, mathematics cannot be dismissed as merely a new form of literature or religion. Nevertheless, many mathematical objects can be seen as shared ideas, like Moby Dick in literature, or the Immaculate Conception in religion.

We entirely subscribe to points 2, 3, and 4, and with certain caveats about objective knowledge[7] to points 1 and 5. In any event mathematics is and will remain a uniquely human undertaking.

This form of humanism sits fairly comfortably with current versions of *social-constructivism*:

> The social constructivist thesis is that mathematics is a social construction, a cultural product, fallible like any other branch of knowledge. (Paul Ernest [127])

[5]That Frege's view of mathematics is wrong, for Hersh as for us, does not diminish its historical importance.

[6]Especially, since a new implementation by Seymour, Robertson, and Thomas in 1997 which has produced a simpler, clearer, and less troubling implementation.

[7]While it is not Hersh's intention, a superficial reading of point 5 hints at a cultural relativism to which we certainly do not subscribe.

We personally qualify this with "Yes, but much less fallible than most." Associated most notably with the writings of Paul Ernest—an English mathematician and professor in the philosophy of mathematics education who carefully traces the intellectual pedigree for his thesis, a pedigree that encompasses the writings of Wittgenstein, Lakatos, Davis, and Hersh among others—social constructivism seeks to define mathematical knowledge and epistemology through the social structure and interactions of the mathematical community and society as a whole.

This interaction often takes place over very long periods. Many of the ideas our students—and some colleagues—take for granted took a great deal of time to gel. The Greeks suspected the impossibility of the three *classical construction problems*,[8] and the irrationality of the golden mean was well known to the Pythagoreans.

While concerns about potential and completed infinities are very old, until the advent of the calculus with Newton and Leibniz and the need to handle fluxions or infinitesimals, the level of need for rigour remained modest. Certainly Euclid is in its geometric domain generally a model of rigour, while also Archimedes' numerical analysis was not equalled until the nineteenth century.

The need for rigour arrives in full force in the time of Cauchy and Fourier. The treacherous countably infinite processes of analysis and the limitations of formal manipulation came to the fore. It is difficult with a modern sensibility to understand how Cauchy's proof of the continuity of pointwise limits could coexist for half a century with Fourier's clear counterexamples originating in his theory of heat.

By the end of the nineteenth century Frege's (1848–1925) attempt to base mathematics in a linguistically based *logicism* had foundered on Russell and other's discoveries of the paradoxes of naive set theory. Within thirty-five years Gödel—and then Turing's more algorithmic treatment[9]—had similarly damaged both Russell and Whitehead's and Hilbert's programs.

Throughout the twentieth century, bolstered by the armour of abstraction, the great ship Mathematics has sailed on largely unperturbed. During the last decade of the nineteenth and first few decades of the twentieth century, the following main streams of philosophy emerged explicitly within mathematics to replace logicism, but primarily as the domain of philosophers and logicians.

[8]Trisection, circle squaring, and cube doubling were taken by the educated to be impossible in antiquity. Already in 414 BCE, in his play *The Birds*, Aristophanes uses "circle-squarers" as a term for those who attempt the impossible. Similarly, the French Academy stopped accepting claimed proofs a full two centuries before the nineteenth century achieved proofs of their impossibility.

[9]The modern treatment of incompleteness leans heavily on Turing's analysis of the *Halting problem* for so-called Turing machines.

- **Platonism.** Everyman's idealist philosophy—stuff exists and we must find it. Despite being the oldest mathematical philosophy, Platonism—still predominant among working mathematicians—was only christened in 1936.

- **Formalism.** Associated mostly with Hilbert—it asserts that mathematics is invented and is best viewed as formal symbolic games without intrinsic meaning.

- **Intuitionism.** Invented by Brouwer and championed by Heyting, intuitionism asks for inarguable monadic components that can be fully analyzed and has many variants; this has interesting overlaps with recent work in cognitive psychology such as Lakoff and Nunez' work, [190], on "embodied cognition".[10] Perhaps that is why the Poincaré conjecture has taken a century to settle [226].

- **Constructivism.** Originating with Markov and especially Kronecker (1823–1891), and refined by Bishop, it finds fault with significant parts of classical mathematics. Its "I'm from Missouri, tell me how big it is" sensibility is not to be confused with Paul Ernest's "social constructivism" [127].

The last two philosophies deny the principle of the *excluded middle*, "*A* or not *A*," and resonate with computer science—as does some of formalism. It is hard after all to run a deterministic program which does not know which disjunctive gate to follow. By contrast the battle between a Platonic idealism (a deductive absolutism) and various forms of fallibilism (a quasi-empirical relativism) plays out across all four, but fallibilism perhaps lives most easily within a restrained version of intuitionism which looks for "intuitive arguments" and is willing to accept that "a proof is what convinces." As Lakatos shows, an argument convincing a hundred years ago may well now be viewed as inadequate. And one today trusted may be challenged in the next century.

As we illustrate in the next section or two, it is only perhaps in the last twenty-five years, with the emergence of powerful mathematical platforms, that any approach other than a largely undigested Platonism and a reliance on proof and abstraction has had the tools[11] to give it traction with working mathematicians.

In this light, Hales' proof of Kepler's conjecture [157] that *the densest way to stack spheres is in a pyramid* resolves the oldest problem in discrete geometry. It also supplies the most interesting recent example of intensively

[10]"The mathematical facts that are worthy of study are those that, by their analogy with other facts are susceptible of leading us to knowledge of a mathematical law, in the same way that physical facts lead us to a physical law" reflects the cognate views of Henri Poincaré (1854–1912) [233, p. 23] on the role of the *subliminal*. He also wrote "It is by logic we prove, it is by intuition that we invent" [232].

[11]That is, to broadly implement Hersh's central points (2-4).

computer-assisted proof, and after five years with the review process was published in the *Annals of Mathematics*—with an "only 99% checked" disclaimer.

This process has triggered very varied reactions [184] and has provoked Thomas Hales to attempt a formal computational proof [241]. Famous earlier examples of fundamentally computer-assisted proof include the *Four color theorem* and proof of the *Nonexistence of a projective plane of order 10*. The three raise and answer quite distinct questions about computer assisted proof—both real and specious.

To make the case as to how far mathematical computation has come, we trace the changes over the past half century. The 1949 computation of π to 2,037 places, suggested by von Neumann, took 70 hours on the original ENIAC. A billion digits may now be computed in much less time on a laptop. Strikingly, it would have taken roughly 100,000 ENIACs to store a modern digital photo—such as the Smithsonian's picture of the ENIAC itself in [50, p. 135]—as is possible thanks to *40 years of Moore's law* in action.

Moore's Law is now taken to be the assertion that *semiconductor technology approximately doubles in capacity and performance roughly every 18 to 24 months*. This is an astounding record of sustained exponential progress without peer in the history of technology. Additionally, mathematical tools are now being implemented on parallel platforms, providing *much* greater power to the research mathematician. Amassing huge amounts of processing power will not alone solve many mathematical problems. There are very few mathematical "Grand-challenge problems" where, as in the physical sciences, a few more orders of computational power will resolve a problem, [54]. There is, however, much more value in *very rapid "Aha's"* as can be obtained through "micro-parallelism"; that is, where we benefit by being able to compute many simultaneous answers on a neurologically rapid scale and so can hold many parts of a problem in our mind at one time.

To sum up, in light of the discussion and terms above, we now describe ourselves as social-constructivists, and as computer-assisted fallabilists with constructivist leanings. We believe that more-and-more the interesting parts of mathematics will be less-and-less susceptible to classical deductive analysis and that Hersh's "nontraditional standard of rigor" must come to the fore.

1.5 Our Experimental Mathodology

Despite Picasso's complaint that "computers are useless, they only give answers," the main goal of computation in pure mathematics is arguably to yield *insight*. This demands speed or, equivalently, substantial *micro-parallelism* to provide answers on a cognitively relevant scale; so that we may ask and answer more questions while they remain in our consciousness. This is relevant for rapid verification; for validation; for *proofs* and *especially for refutations* which includes what Lakatos calls "monster barring" [189]. Most of this goes on in the daily small-scale accretive level of mathematical discovery but insight is gained even in cases like the proof of the four color theorem or the nonexistence of a plane of order ten. Such insight is not found in the case-enumeration of the proof, but rather in the algorithmic reasons for believing that one has at hand a tractable unavoidable set of configurations or another effective algorithmic strategy.

In this setting it is enough to equate *parallelism* with access to requisite *more* space and speed of computation. Also, we should be willing to consider all computations as "exact" which provide truly reliable answers.[12] This now usually requires a careful *hybrid* of symbolic and numeric methods, such as achieved by *Maple*'s liaison with the Numerical Algorithms Group (NAG) Library,[13] see [48, 275]. There are now excellent tools for such purposes throughout analysis, algebra, geometry, and topology; see [50, 51, 54, 64, 275].

Along the way questions required by—or just made natural by—computing start to force out older questions and possibilities in the way beautifully described a century ago by Dewey regarding evolution [119].

> Old ideas give way slowly; for they are more than abstract logical forms and categories. They are habits, predispositions, deeply engrained attitudes of aversion and preference. Moreover, the conviction persists—though history shows it to be a hallucination—that all the questions that the human mind has asked are questions that can be answered in terms of the alternatives that the questions themselves present. But in fact intellectual progress usually occurs through sheer abandonment of questions together with both of the alternatives they assume; an abandonment that results from their decreasing vitality and a change of urgent interest. We do not solve them: we get over them. Old questions are solved by disappearing, evaporating, while new questions corresponding to the changed attitude of endeavor and preference take their place. Doubtless the greatest dissolvent in contemporary thought of old questions, the greatest precipitant of new methods, new intentions, new problems, is the one effected by the scientific revolution that found its climax in the "Origin of Species." (John Dewey)

[12]If careful interval analysis can certify that a number known to be an integer is larger than 2.5 and less than 3.5, this constitutes a exact computational proof that it is 3.

[13]See [223] http://www.nag.co.uk/.

Additionally, what is "easy" changes: high performance computing and networking are blurring, merging disciplines and collaborators. This is democratizing mathematics but further challenging authentication—consider how easy it is to find information on *Wikipedia*[14] and how hard it is to validate it.

Moving towards a well-articulated Experimental *Mathodology*—both in theory and practice—will take much effort. The need is premised on the assertions that intuition is acquired—we can and must better mesh computation and mathematics, and that visualization is of growing importance—in many settings even three is a lot of dimensions.

"Monster-barring" (Lakatos's term [189] for refining hypotheses to rule out nasty counter-examples[15]) and "caging" (our own term for imposing needed restrictions in a conjecture) are often easy to enhance computationally, as for example with randomized checks of equations, linear algebra, and primality or graphic checks of equalities, inequalities, areas, etc.

1.5.1 Eight Roles for Computation

We next recapitulate eight roles for computation as discussed by two of the current authors (D. Bailey and J. Borwein) in their two recent books [50, 51]:

1. *Gaining insight and intuition, or just knowledge*. Working algorithmically with mathematical objects almost inevitably adds insight to the processes one is studying. At some point even just the careful aggregation of data leads to better understanding.

2. *Discovering new facts, patterns, and relationships*. The number of *additive partitions* of a positive integer n, $p(n)$, is *generated* by

$$1+\sum_{n\geq 1} p(n)q^n = \prod_{n=1}^{\infty}(1-q^n)^{-1}. \tag{1.2}$$

Thus, $p(5) = 7$ since

$$\begin{aligned} 5 &= 4+1 = 3+2 = 3+1+1 \\ &= 2+2+1 = 2+1+1+1 = 1+1+1+1+1. \end{aligned} \tag{1.3}$$

Developing (1.2) is a fine introduction to enumeration via *generating functions*. Additive partitions are harder to handle than multiplicative factorizations, but they are very interesting [51, Chapter 4]. Ramanujan used Major

[14] *Wikipedia* is an open source project [280]; "wiki-wiki" is Hawaiian for "quickly."

[15] Is, for example, a polyhedron always convex? Is a curve intended to be simple? Is a topology assumed Hausdorff, a group commutative?

MacMahon's table of $p(n)$ to intuit remarkable deep congruences such as

$$p(5n+4) \equiv 0 \mod 5,\ p(7n+5) \equiv 0 \mod 7,$$

and

$$p(11n+6) \equiv 0 \mod 11,$$

from relatively limited data like

$$\begin{aligned} P(q) = 1 + q + 2q^2 + 3q^3 + \underline{5}\,q^4 + \overline{7}\,q^5 + 11\,q^6 + 15\,q^7 \\ + 22\,q^8 + \underline{30}\,q^9 + 42\,q^{10} + 56\,q^{11} + \overline{77}\,q^{12} + 101\,q^{13} \\ + \underline{135}\,q^{14} + 176\,q^{15} + 231\,q^{16} + 297\,q^{17} + 385\,q^{18} \\ + \overline{\underline{490}}\,q^{19} + 627\,q^{20}b + 792\,q^{21} + 1002\,q^{22} + \cdots. \end{aligned} \tag{1.4}$$

Cases $5n+4$ and $7n+5$ are flagged in (1.4). Of course, it is markedly easier to (heuristically) confirm than find these fine examples of *Mathematics: The Science of Patterns*.[16] The study of such congruences—much assisted by symbolic computation—is very active today.

3. *Graphing to expose mathematical facts, structures or principles.* Consider Nick Trefethen's fourth challenge problem as described in [48, 275]. It requires one to find ten good digits of:

   What is the global minimum of the function

$$\begin{aligned} e^{\sin(50x)} + \sin(60e^y) + \sin(70\sin x) \\ + \sin(\sin(80y)) - \sin(10(x+y)) + (x^2+y^2)/4? \end{aligned} \tag{1.5}$$

   As a foretaste of future graphic tools, one can solve this problem graphically and interactively using current *adaptive 3-D plotting* routines which can catch all the bumps. This does admittedly rely on trusting a good deal of software.

4. *Rigourously testing and especially falsifying conjectures.* We hew to the Popperian scientific view that we primarily falsify; but that as we perform more and more testing experiments without such falsification, we draw closer to firm belief in the truth of a conjecture such as *the polynomial* $P(n) = n^2 - n + p$ *has prime values for all* $n = 0, 1, \ldots, p-2$, *exactly for* Euler's lucky prime numbers, *that is, p= 2, 3, 5, 11, 17, and 41.*[17]

[16] The title of Keith Devlin's 1996 book [118].
[17] See [279] for the answer.

5. *Exploring a possible result to see if it* merits *formal proof*. A conventional deductive approach to a hard multistep problem really requires establishing all the subordinate lemmas and propositions needed along the way, especially if they are highly technical and unintuitive. Now some may be independently interesting or useful, but many are only worth proving if the entire expedition pans out. Computational experimental mathematics provides tools to survey the landscape with little risk of error: Only if the view from the summit is worthwhile does one lay out the route carefully. We discuss this further at the end of the next section.

6. *Suggesting approaches for formal proof*. The proof of the *cubic theta function identity* discussed on [51, pp. 210] shows how a fully intelligible human proof can be obtained entirely by careful symbolic computation.

7. *Computing replacing lengthy hand derivations*. Who would wish to verify the following prime factorization by hand?

$$\begin{aligned}&6422607578676942838792549775208734746307\\&= (2140992015395526641)(1963506722254397)(1527791).\end{aligned}$$

   Surely, what we value is understanding the underlying algorithm, not the human work?

8. *Confirming analytically derived results*. This is a wonderful and frequently accessible way of confirming results. Even if the result itself is not computationally checkable, there is often an accessible corollary. An assertion about bounded operators on Hilbert space may have a useful consequence for three-by-three matrices. It is also an excellent way to error correct, or to check calculus examples before giving a class.

1.6 Finding Things versus Proving Things

We now illuminate these eight roles with eight mathematical examples. At the end of each we note some of the roles illustrated.

Example 1.1 (Pictorial Comparison). Pictorially comparing $y - y^2$ and $y^2 - y^4$ to $-y^2\log(y)$, when y lies in the unit interval, is a much more rapid way to divine which function is larger than by using traditional analytic methods.

Figure 1.2 shows that it is clear in the later case that the functions cross, and so it is futile to try to prove one majorizes the other. In the first case, evidence is

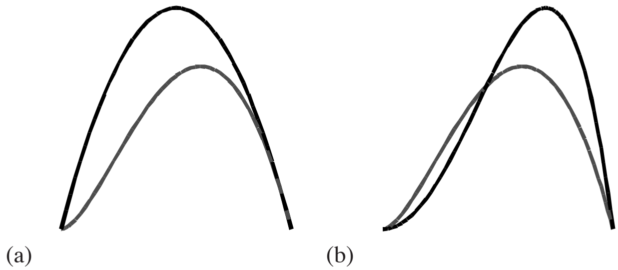


Figure 1.2. Graphical comparison of (a) $y-y^2$ and (b) y^2-y^4 to $-y^2\log(y)$.

provided to motivate attempting a proof and often the picture serves to guide such a proof—by showing monotonicity or convexity or some other salient property. ◇

This certainly illustrates roles 3 and 4, and perhaps role 5.

Example 1.2 (A Proof and a Disproof). Any modern computer algebra system can tell one that

$$0 < \int_0^1 \frac{(1-x)^4 x^4}{1+x^2}\,dx = \frac{22}{7} - \pi, \tag{1.6}$$

since the integral may be interpreted as the area under a positive curve. We are however no wiser as to why! If however we ask the same system to compute the indefinite integral, we are likely to be told that

$$\int_0^t \cdot = \frac{1}{7}t^7 - \frac{2}{3}t^6 + t^5 - \frac{4}{3}t^3 + 4t - 4\arctan(t).$$

Then (1.6) is now rigourously established by differentiation and an appeal to the Fundamental Theorem of Calculus. ◇

This illustrates roles 1 and 6. It also falsifies the bad conjecture that $\pi = 22/7$ and so illustrates role 4 again. Finally, the computer's proof is easier (role 7) and very nice, though probably it is not the one we would have developed by ourselves. The fact that $22/7$ is a continued fraction approximation to π has lead to many hunts for generalizations of (1.6), see [51, Chapter 1]. None so far are entirely successful.

Example 1.3 (Computer Discovery and 'Proof' of the Series for $\mathbf{arcsin^2(x)}$). We compute a few coefficients and observe that there is a regular power of 4 in the numerator, and integers in the denominator; or equivalently we look at

$\arcsin(x/2)^2$. In the following code, the generating function package `gfun` in *Maple* then predicts a recursion, r, for the denominators and solves it, as R:

```
with(gfun):
s:=[seq(1/coeff(series(arcsin(x/2)^2,x,25),x,2*n),n=1..6)];
R:=unapply(rsolve(op(1, listtorec(s,r(m))),r(m)),m);
[seq(R(m),m=0..8)];
```

This yields $s := [4, 48, 360, 2240, 12600, 66528]$ and

$$R := m \mapsto 8\,\frac{4^m\,\Gamma(3/2+m)(m+1)}{\pi^{1/2}\Gamma(1+m)},$$

where Γ is the Gamma function (as ususal, $\Gamma(x) := \int_0^\infty t^{x-1}\,e^{-t}\,dt$, which we will discuss more fully in Chapter 7 but will use throughout), and then returns the sequence of values

$$[4, 48, 360, 2240, 12600, 66528, 336336, 1647360, 7876440].$$

We may now use Sloane's *Online Encyclopedia of Integer Sequences* [255] to reveal that the coefficients are $R(n) = 2n^2\binom{2n}{n}$. More precisely, sequence A002544 identifies

$$R(n+1)/4 = \binom{2n+1}{n}(n+1)^2.$$

The command

```
[seq(2*n^2*binomial(2*n,n),n=1..8)];
```

confirms this with

$$[4, 48, 360, 2240, 12600, 66528, 336336, 1647360].$$

Next we write

```
S:=Sum((2*x)^(2*n)/(2*n^2*binomial(2*n,n)),n=1..infinity):
S=value(S);
```

which returns

$$\frac{1}{2}\sum_{n=1}^{\infty}\frac{(2x)^{2n}}{n^2\binom{2n}{n}} = \arcsin^2(x).$$

That is, we have discovered—and proven if we trust or verify *Maple*'s summation algorithm—the desired Maclaurin series.

As prefigured by Ramanujan, it transpires that there is a beautiful closed form for $\arcsin^{2m}(x)$ for all $m = 1, 2, \ldots$. In [63] there is a discussion of the use of *integer relation methods*, [50, Chapter 6], to find this closed form and associated proofs are presented; some information is also given in the exercises below. ◇

Here we see an admixture of all of the roles save role 3, but above all roles 2 and 5.

Example 1.4 (Discovery without Proof). Donald Knuth[18] asked for a closed form evaluation of

$$\sum_{k=1}^{\infty}\left\{\frac{k^k}{k!\,e^k}-\frac{1}{\sqrt{2\pi k}}\right\} \quad = \quad -0.084069508727655\ldots. \tag{1.7}$$

Since about 2000 CE it has been easy to compute 20—or 200—digits of this sum. Now the *Inverse Symbolic Calculator* (ISC) at [84] http://oldweb.cecm.sfu.ca/projects/ISC/ uses a variety of search algorithms and heuristics to predict what a number might actually be.[19] Similar ideas are now implemented as `identify` in *Maple* and `Recognize` in *Mathematica*, and are described in [27,48,50,64]. In this case it returns

$$0.084069508727655 \approx \frac{2}{3}+\frac{\zeta(1/2)}{\sqrt{2\pi}}.$$

We thus have a prediction which *Maple* 9.5 on a 2004 laptop *confirms* to 100 places in under 6 seconds and to 500 in 40 seconds. Arguably we are done. After all we were asked to *evaluate* the series and we now know a closed-form answer. Notice also that the 'divergent' $\zeta(1/2)$ term is formally to be expected! ◇

We have discovered and tested the result and in so doing gained insight and knowledge while illustrating roles 1, 2, and 4. Moreover, as described in [51, pp. 15], one can also be lead by the computer to a very satisfactory computer-assisted but very human proof, thus illustrating role 6. Indeed, the first hint is that the computer algebra system returned the value in (1.7) very quickly even though the series is very slowly convergent. This suggests the program is doing something intelligent—and it is!

Example 1.5 (A Striking Conjecture with No Known Proof Strategy). For $N = 1,2,3,\ldots,$

$$8^N\,\zeta\left(\{-2,1\}_N\right) \stackrel{?}{=} \zeta\left(\{2,1\}_N\right). \tag{1.8}$$

Explicitly, the first two cases are

$$8\sum_{n>m>0}\frac{(-1)^n}{n^2m} \quad = \quad \sum_{n>m>0}\frac{1}{n^2m} = \sum_{n>0}\frac{1}{n^3},$$

$$64\sum_{n>m>o>p>0}\frac{(-1)^n(-1)^o}{n^2mo^2p} \quad = \quad \sum_{n>m>o>p>0}\frac{1}{n^2mo^2p} = \sum_{n>m>0}\frac{1}{n^3m^3},$$

[18] Posed as an MAA Problem [181].

[19] The ISC is currently being rebuilt and brought up to date.

where the problem lies in the left-hand identities. The notation should now be clear—the curly brackets denote a repetition and negative entries an alternation. Such alternating sums are called *multivariate zeta values* (MZV), and positive ones are called *Euler sums* after Euler who first studied them seriously. They arise naturally in a variety of modern fields from combinatorics to mathematical physics and knot theory. Some more discussion of them will be given in Chapters 2 and 8.

There is abundant evidence amassed since "identity" (1.8) was found in 1996. For example, very recently Petr Lisoněk checked the first 85 cases to 1000 places in about 41 HP hours with only the *predicted round-off error*. And the case $N = 163$ was checked in about ten hours. These objects are very hard to compute naively and require substantial computation as a precursor to their analysis.

Formula (1.8) is the *only* identification of its type of an Euler sum with a distinct MZV and we have no idea why it is true. Any similar MZV proof has been both highly nontrivial and illuminating. To illustrate how far we are from proof: Can just the case $N = 2$ be proven *symbolically* as has been the case for $N = 1$? ◇

This identity was discovered by the British quantum field theorist David Broadhurst and J. Borwein during a large hunt for such objects in the mid-nineties. In this process the authors discovered and proved many lovely results (see [50, Chapter 2] and [51, Chapter 4]), thereby illustrating roles 1, 2, 4, 5, and 7. In the case of identity (1.8) the authors have failed with role 6, but have ruled out many sterile approaches. It is one of many examples where we can now have (near) certainty without proof. Another was shown in (1.1).

Example 1.6 (What You Draw *Is* What You See). As the quote in the caption of Figure 1.3 suggests, pictures are highly metaphorical. Figure 1.3 shows roots of polynomials with coefficients 1 or –1 up to degree 18. The colouration is determined by a normalized sensitivity of the coefficients of the polynomials to slight variations around the values of the zeroes with red indicating low sensitivity and violet indicating high sensitivity. It is hard to see how the structure revealed in the pictures above[20] would be seen other than through graphically data-mining. Note the different shapes—now proven—of the holes around the various roots of unity.

The striations are unexplained but all recomputations expose them! And the fractal structure is provably there. Nonetheless different ways of measuring the stability of the calculations reveal somewhat different features. This is very much analogous to a chemist discovering an unexplained but robust spectral line. ◇

[20]We plot all complex zeroes of polynomials with only –1 and 1 as coefficients up to a given degree. As the degree increases some of the holes fill in—at different rates.

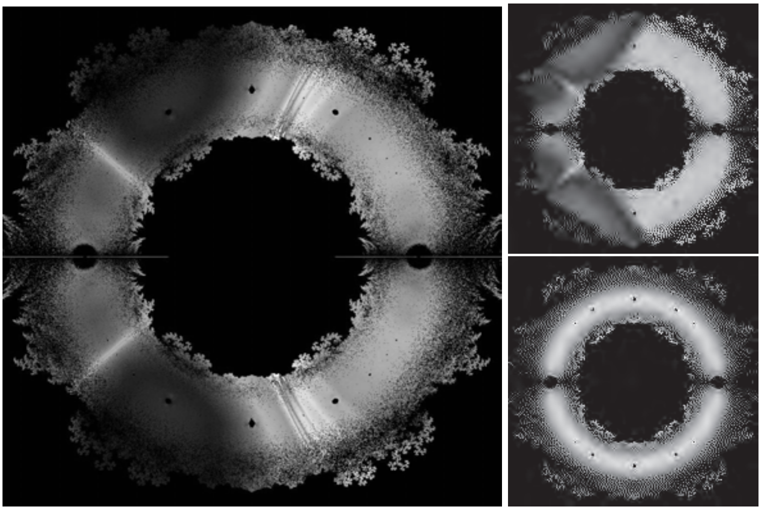


Figure 1.3. "The price of metaphor is eternal vigilance." (Arturo Rosenblueth & Norbert Wiener [200])

This certainly illustrates role 2 and role 7, but also roles 1 and 3.

Example 1.7 (Visual Dynamics). In recent continued fraction work, Crandall and J. Borwein needed to study the *dynamical system* $t_0 := t_1 := 1$:

$$t_n \hookleftarrow \frac{1}{n} t_{n-1} + \omega_{n-1} \left(1 - \frac{1}{n}\right) t_{n-2},$$

where $\omega_n = a^2$ for n even and $\omega_n = b^2$ for n odd, lie on the unit circle in $\mathbb{C}$. Think of this as a *black box* which we wish to examine scientifically. Numerically, all one *sees* is $t_n \to 0$ slowly. Pictorially, we *learn* significantly more.[21] If the iterates are plotted with colour changing after every few hundred iterates, it is clear that they spiral roman-candle like in to the origin, see Figure 1.4.

Scaling by $\sqrt{n}$, and coloring even and odd iterates, *fine structure* appears; see Figure 1.5. We now observe, predict, and validate that the outcomes depend on whether or not one or both of a and b are roots of unity. Input a p-th root of unity and out come p points attracting iterates, input a nonroot of unity and we see a circle. ◇

This forceably illustrates role 2 but also roles 1, 3, and 4. It took one of the current authors (J. Borwein) and his coauthors over a year and 100 pages to

[21]... "Then felt I like a watcher of the skies, when a new planet swims into his ken." (Chapman's *Homer*)

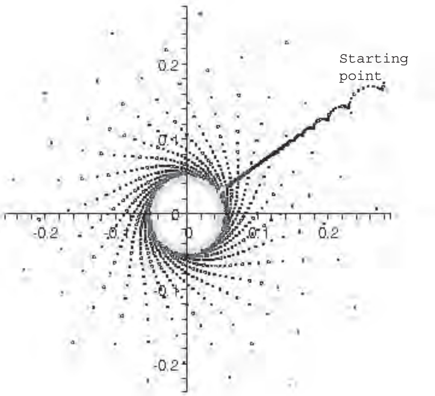


Figure 1.4. Visual convergence in the complex plane.

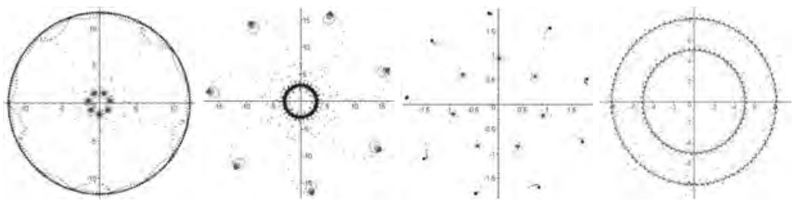


Figure 1.5. The attractors for various $|a| = |b| = 1$.

convert this intuition into a rigorous formal proof [13]. Indeed, the results are technical and delicate enough that we have more faith in the facts than in the finished argument. In this sentiment, we are not entirely alone.

Carl Friedrich Gauss, who drew (carefully) and computed a great deal, once noted, "I *have* the result, but I do not yet know how to get it."[22] An excited young Gauss writes: "A new field of analysis has appeared to us, self-evidently, in the study of functions etc" (October 1798). It and the consequent proofs pried open the doors of much modern elliptic function and number theory.

Our penultimate and more comprehensive example is more sophisticated and we beg the less-expert analyst's indulgence. Please consider its structure and not the details.

Example 1.8 (A Full Run). Consider the *unsolved* Problem 10738 from the 1999 *American Mathematical Monthly* [51]:

[22]Likewise, the quote has so far escaped exact isolation!

Problem. For $t > 0$ let

$$m_n(t) = \sum_{k=0}^{\infty} k^n \exp(-t)\,\frac{t^k}{k!}$$

be the nth moment of a *Poisson distribution* with parameter t. Let $c_n(t) = m_n(t)/n!$. Show

(a) $\{m_n(t)\}_{n=0}^{\infty}$ is log-convex[23] for all $t > 0$.

(b) $\{c_n(t)\}_{n=0}^{\infty}$ is not log-concave for $t < 1$.

(c*) $\{c_n(t)\}_{n=0}^{\infty}$ is log-concave for $t \geq 1$.

Solution. (a) Neglecting the factor of $\exp(-t)$ as we may, this reduces to

$$\sum_{k,j\geq 0} \frac{(jk)^{n+1}t^{k+j}}{k!\,j!} \leq \sum_{k,j\geq 0} \frac{(jk)^n t^{k+j}}{k!\,j!}\,k^2 = \sum_{k,j\geq 0} \frac{(jk)^n t^{k+j}}{k!\,j!}\,\frac{k^2+j^2}{2},$$

and this now follows from $2jk \leq k^2 + j^2$.

(b) As

$$m_{n+1}(t) = t\sum_{k=0}^{\infty}(k+1)^n \exp(-t)\,\frac{t^k}{k!},$$

on applying the binomial theorem to $(k+1)^n$, we see that $m_n(t)$ satisfies the recurrence

$$m_{n+1}(t) = t\sum_{k=0}^{n}\binom{n}{k} m_k(t), \qquad m_0(t) = 1.$$

In particular for $t = 1$, we computationally obtain as many terms of the sequence

$$1, 1, 2, 5, 15, 52, 203, 877, 4140\ldots$$

as we wish. These are the *Bell numbers* as was discovered again by consulting *Sloane's Encyclopedia* which can also tell us that, for $t = 2$, we have the *generalized Bell numbers*, and gives the exponential generating functions.[24] Inter alia, an explicit computation shows that

$$t\,\frac{1+t}{2} = c_0(t)\,c_2(t) \leq c_1(t)^2 = t^2$$

exactly if $t \geq 1$, which completes (b).

[23] A sequence $\{a_n\}$ is *log-convex* if $a_{n+1}a_{n-1} \geq a_n^2$ for $n \geq 1$, and log-concave when the sign is reversed.

[24] Bell numbers were known earlier to Ramanujan—an example of *Stigler's Law of Eponymy* [51, p. 60].

Also, preparatory to the next part, a simple calculation shows that

$$\sum_{n\geq 0} c_n u^n = \exp\left(t(e^u - 1)\right). \tag{1.9}$$

We appeal to a recent theorem due to E. Rodney Canfield [51] which proves the lovely and quite difficult result below. A self-contained proof would be very fine.

Theorem 1.9. *If a sequence* $1, b_1, b_2, \cdots$ *is nonnegative and log-concave then so is the sequence* $1, c_1, c_2, \cdots$ *determined by the generating function equation*

$$\sum_{n\geq 0} c_n u^n = \exp\left(\sum_{j\geq 1} b_j \frac{u^j}{j}\right).$$

Using equation (1.9) above, we apply this to the sequence $b_j = t/(j-1)!$ which is log-concave exactly for $t \geq 1$. $\diamond$

A search in 2001 on *MathSciNet* for "Bell numbers" since 1995 turned up 18 items. Canfield's paper showed up as number 10. Later, *Google* found it immediately!

Quite unusually, the given solution to (c) was the only one received by the *Monthly*. The reason might well be that it relied on the following sequence of steps:

A **(Question Posed)** ⇒ Computer Algebra System ⇒ Interface ⇒
Search Engine ⇒ Digital Library ⇒ Hard New Paper ⇒ **(Answer)**

Without going into detail, we have visited most of the points elaborated in Section 1.4.1. Now if only we could already automate this process!

Jacques Hadamard describes the role of proof as well as anyone—and most persuasively given that his 1896 proof of the Prime number theorem is an inarguable apex of rigorous analysis.

> The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it.[25]
> (Jacques Hadamard)

Of the eight uses of computers instanced above, let us reiterate the central importance of heuristic methods for determining what is true and whether it merits proof. We tentatively offer the following surprising example which is very very likely to be true, offers no suggestion of a proof and indeed may have no reasonable proof.

[25]Hadamard quoted in [234]. See also [233].

Example 1.10 (The Hexadecimal Expansion of π).
Conjecture. *Consider* $x_0 = 0$ *and, for* $n > 0$,

$$x_n = \left\{ 16x_{n-1} + \frac{120n^2 - 89n + 16}{512n^4 - 1024n^3 + 712n^2 - 206n + 21} \right\}. \tag{1.10}$$

The sequence $\beta_n = (\lfloor 16x_n \rfloor)$, *where* (x_n) *is the sequence of iterates defined in equation (1.10), precisely generates the hexadecimal expansion of* $\pi - 3$.

(Here $\{\cdot\}$ denotes the fractional part and $(\lfloor\cdot\rfloor)$ denotes the integer part.) In fact, we know from [50, Chapter 4] that the first million iterates are correct and in consequence we can consider the sum

$$\sum_{n=1,000,000}^{\infty} |x_{n+1} - \{16^n \pi\}| \leq 1.465 \times 10^{-7} \ldots . \tag{1.11}$$

By the first Borel-Cantelli lemma this shows that the hexadecimal expansion of π only finitely differs from (β_n). Heuristically, the probability of any error is very low. ◇

1.7 Conclusions

To summarize, we do argue that reimposing the primacy of mathematical knowledge over proof is appropriate. So we return to the matter of what it takes to persuade an individual to adopt new methods and drop time honoured ones. Aptly, we may start by consulting Kuhn on the matter of paradigm shift:

> The issue of paradigm choice can never be unequivocally settled by logic and experiment alone.... in these matters neither proof nor error is at issue. The transfer of allegiance from paradigm to paradigm is a conversion experience that cannot be forced.[26] (Thomas Kuhn)

As we have seen, the pragmatist philosopher John Dewey eloquently agrees, while Max Planck [231] has also famously remarked on the difficulty of such paradigm shifts. This is Kuhn's version:[27]

> And Max Planck, surveying his own career in his Scientific Autobiography, sadly remarked that "a new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die, and a new generation grows up that is familiar with it." (Albert Einstein [188, 231])

[26] In [247], *Who Got Einstein's Office?* The answer is Arne Beurling.

[27] Kuhn is quoting Einstein quoting Planck. There are various renderings of this second-hand German quotation.

This transition is certainly already apparent. It is certainly rarer to find a mathematician under thirty who is unfamiliar with at least one of *Maple*, *Mathematica* or *Matlab*, than it is to find one over sixty-five who is really fluent. As such fluency becomes ubiquitous, we expect a rebalancing of our community's valuing of deductive proof over inductive knowledge.

In his "*Mathematische Probleme*" lecture to the Paris International Congress in 1900, Hilbert writes[28]

> Moreover a mathematical problem should be difficult in order to entice us, yet not completely inaccessible, lest it mock our efforts. It should be to us a guidepost on the mazy path to hidden truths, and ultimately a reminder of our pleasure in the successful solution. (David Hilbert)

Note the primacy given by a most exacting researcher to discovery and to truth over proof and rigor. More controversially and most of a century later, Greg Chaitin invites us to be bolder and act more like physicists.

> I believe that elementary number theory and the rest of mathematics should be pursued more in the spirit of experimental science, and that you should be willing to adopt new principles.... And the Riemann Hypothesis isn't self-evident either, but it's very useful. A physicist would say that there is ample experimental evidence for the Riemann Hypothesis and would go ahead and take it as a working assumption.... We may want to introduce it formally into our mathematical system. (Greg Chaitin [50, p. 254])

Ten years later:

> [Chaitin's] "Opinion" article proposes that the Riemann hypothesis (RH) be adopted as a new axiom for mathematics. Normally one could only countenance such a suggestion if one were assured that the RH was undecidable. However, a proof of undecidability is a logical impossibility in this case, since if RH is false it is provably false. Thus, the author contends, one may either wait for a proof, or disproof, of RH—both of which could be impossible—or one may take the bull by the horns and accept the RH as an axiom. He prefers this latter course as the more positive one. (Roger Heath-Brown[29])

[28]See the late Ben Yandell's fine account of the Hilbert Problems and their solvers [286]. The written lecture is considerably longer and further ranging that the one delivered in person.

[29]Roger Heath-Brown's *Mathematical Review* of [86], 2004.

Much as we admire the challenge of Greg Chaitin's statements, we are not yet convinced that it is helpful to add axioms as opposed to proving conditional results that start "Assuming the continuum hypothesis" or emphasize that "without assuming the Riemann hypothesis we are able to show." Most important is that we lay our cards on the table. We should explicitly and honestly indicate when we believe our tools to be heuristic, we should carefully indicate why we have confidence in our computations—and where our uncertainty lies—and the like.

On that note, Hardy is supposed to have commented (somewhat dismissively) that Landau, a great German number theorist, would never be the first to prove the Riemann Hypothesis, but that if someone else did so then Landau would have the best possible proof shortly after. We certainly hope that a more experimental methodology will better value independent replication and honour the first transparent proof[30] of Fermat's last theorem as much as Andrew Wiles' monumental proof. Hardy also commented that he did his best work past forty. Inductive, accretive, tool-assisted mathematics certainly allows brilliance to be supplemented by experience and—as in our case—stands to further undermine the notion that one necessarily does ones best mathematics young.

1.7.1 Last Words

To reprise, we hope to have made convincing arguments that the traditional deductive accounting of Mathematics is a largely ahistorical caricature—Euclid's millennial sway not withstanding.[31] Above all, mathematics is primarily about *secure knowledge* not proof, and that while the aesthetic is central, we must put much more emphasis on notions of supporting evidence and attend more closely to the reliability of witnesses.

Proofs are often out of reach—but understanding, even certainty, is not. Clearly, computer packages can make concepts more accessible. A short list includes linear relation algorithms, Galois theory, Groebner bases, etc. While progress is made "one funeral at a time,"[32] in Thomas Wolfe's words "you can't go home again" and as the coinventor of the fast Fourier transform properly observed

> Far better an approximate answer to the right question, which is often vague, than the exact answer to the wrong question, which can always be made precise. (J. W. Tukey, 1962)

[30] If such should exist and as you prefer be discovered or invented.

[31] Most of the cited quotations are stored at [49] http://users.cs.dal.ca/~jborwein/quotations.html.

[32] This grim version of Planck's comment is sometimes attributed to Niels Bohr but this seems specious. It is also spuriously attributed on the web to Michael Milken, and probably many others.

Now is a wonderful time to be a (computational) mathematician. This is forcibly brought home by the *Business Week* cover story of January 23, 2006, entitled “Math Will Rock Your World.” It comments

> These slices of our lives now sit in databases, many of them in the public domain. From a business point of view, they’re just begging to be analyzed. But even with the most powerful computers and abundant, cheap storage, companies can’t sort out their swelling oceans of data, much less build businesses on them, without enlisting skilled mathematicians and computer scientists. The rise of mathematics is heating up the job market for luminary quants, especially at the Internet powerhouses where new math grads land with six-figure salaries and rich stock deals. Tom Leighton, an entrepreneur and applied math professor at Massachusetts Institute of Technology, says: “All of my students have standing offers at Yahoo! and Google.” Top mathematicians are becoming a new global elite. It’s a force of barely 5,000, by some guesstimates, but every bit as powerful as the armies of Harvard University MBAs who shook up corner suites a generation ago.

2 Algorithms for Experimental Mathematics I

"Great algorithms are the poetry of computation." At the beginning of this century, Sullivan and Dongarra could so write when they compiled a list of the 10 algorithms having "the greatest influence on the development and practice of science and engineering in the 20th century."

—From "Random Samples," *Science*, February 4, 2000[1]

2.1 The Poetry of Computation

Many different computational methods have been used in experimental mathematics. Just a few of the more widely used methods are the following:

1. Symbolic computation for algebraic and calculus manipulations.
2. Integer-relation methods, especially the PSLQ algorithm.
3. High-precision integer and floating-point arithmetic.
4. High-precision evaluation of integrals and infinite series summations.
5. The Wilf-Zeilberger algorithm for proving summation identities.
6. Iterative approximations to continuous functions.
7. Identification of functions based on graph characteristics.
8. Graphics and visualization methods targeted to mathematical objects.

In this chapter and in Chapter 3 we will present an overview of some of these methods, and give examples of how they have been used in some real-world experimental math research. We will focus on items 2, 3, 4, and 5, mainly because the essential ideas can be explained more easily than, say, the mechanics behind symbolic computation or advanced scientific visualization.

[1]The full article appeared in the January/February 2000 issue of *Computing in Science & Engineering*.

2.2 High-Precision Arithmetic

We have already mentioned examples of high-precision numerical calculations such as Petr Lisoněk's numerical test of the first 85 cases of identity (1.8) in Section 1.6. Indeed, such computations frequently arise in experimental mathematics. We shall focus here on high-precision floating-point computation. High-precision integer computation is also required in some aspects of mathematical computation, particularly in prime number computations and symbolic manipulations, but as we shall see, many of the algorithms described below are equally applicable to both types of arithmetic. An excellent presentation of high-precision integer arithmetic is given in [108].

By "arbitrary precision" we mean a software facility that permits one to adjust the level of numeric precision over a wide range, typically extending to the equivalent of thousands or possibly even millions of decimal digits. An extended dynamic range is almost always included as well, since such computations often require a larger range than the $10^{\pm 308}$ range available with the IEEE double format.

For these levels of precision, the best approach is as follows. Define an arbitrary precision datum to be an $(n+4)$-long string of words. The sign of the first word is the sign $\pm$ of the datum, and the absolute value of the first word is n, the number of mantissa words used. The second word contains an exponent p. Words three through $n+2$ are the n mantissa words m_i, each of which has an integer value between 0 and 2^b-1, or in other words b bits of the mantissa. Finally, words $n+3$ and $n+4$ are reserved as "scratch" words for various arithmetic routines. One can optionally designate an additional word, placed at the start of the data structure, to specify the amount of memory available for this datum, so as to avoid memory overwrite errors during execution. The value A represented by this datum is

$$A = \pm(2^{pb}m_1 + 2^{(p-1)b}m_2 + 2^{(p-2)b}m_3 + \cdots + 2^{(p-n+1)b}m_n),$$

where it is assumed that $m_1 \neq 0$ and $m_n \neq 0$ for nonzero A. Zero is represented by a string consisting of a sign word and an exponent word, both of which are zero.

There are several variations possible with this general design. One approach is to utilize 64-bit IEEE floating-point words, with 48 mantissa bits per word. Addition operations can easily be performed by adding the two vectors of mantissas (suitably shifted to adjust for differences in exponent), and then releasing carries beginning from the last mantissa word back to the first. Multiplication and division can be performed by straightforward adaptations of the long multiplication and long division schemes taught in grammar school, performed modulo 2^{48} instead of modulo 10. The multiplication of two individual 48-bit entities can be performed by simple algorithms, or, on some systems, by using the "fused multiply-add" hardware instruction. Up to $2^5 = 32$ such products can be accumulated before needing to release carries, since $5 + 48 = 53$, and integers as large as 2^{53} can be accommodated exactly in a 64-bit IEEE word. This approach was taken in the software package described in [25], and available at the URL [15] http://www.experimentalmath.info. This software includes C++ and Fortran-90 translation modules, so that these functions can be invoked from ordinary programs with only minor modifications to the source code.

Another approach is to utilize arrays of integer data, with integer arithmetic operations, since all values in the data structure above are whole numbers. One disadvantage of this approach is that it is hard to write programs that are both fast and easily portable to different systems. Nonetheless, some integer-based implementations have been very successful, notably the GNU package [145].

Either way, an FFT-based convolution scheme can be used to accelerate multiplication for higher levels of precision (approximately 1000 digits or more). The reason for the savings is that an FFT calculation scales only as $n \log^2 n$ (in a simple approach), respectively $n \log n \log(\log n)$ (in the best-known scheme, the Schönhage-Strassen algorithm) in computational cost, compared to the n^2 for conventional methods (where n is the precision in digits or words). Divisions and square roots can in turn be accelerated by utilizing Newton iterations [50, pp. 223–229].

2.3 Integer Relation Detection

Integer relation detection methods are employed very often in experimental math applications to recognize a mathematical constant whose numerical value can be computed to at least moderately high precision, and also to discover relations between a set of computed numerical values.

For a given real vector $(x_1, x_2, \cdots, x_n)$, an integer relation algorithm is a computational scheme that either finds the n integers $(a_1, a_2, \cdots, a_n)$, not all zero, such that $a_1x_1 + a_2x_2 + \cdots a_nx_n = 0$ or else establishes that there is no such integer vector within a ball of some radius about the origin, where the metric is the Euclidean norm $(a_1^2 + a_2^2 + \cdots + a_n^2)^{1/2}$.

At the present time, the best-known integer relation algorithm is the PSLQ algorithm [135] of Helaman Ferguson. Another widely used integer relation detection scheme involves the Lenstra-Lenstra-Lovasz (LLL) lattice reduction algorithm. The PSLQ algorithm, together with related lattice reduction schemes such as LLL, was recently named one of ten "algorithms of the century" by the publication *Computing in Science and Engineering* [10]. In addition to possessing good numerical stability, PSLQ is guaranteed to find a relation in a polynomially bounded number of iterations. The name "PSLQ" derives from its usage of a partial sum of squares vector and a LQ (lower-diagonal-orthogonal) matrix factorization.

A simplified formulation of the standard PSLQ algorithm, mathematically equivalent to the original formulation, is given in [23] and [50, pp. 230–234]. These references also describe another algorithm, called "multi-pair" PSLQ, which is well-suited for parallel processing, and which runs faster even on a one-CPU system than the standard PSLQ. Two-level and three-level variants of both standard PSLQ and multi-pair PSLQ, which economize on runtime by performing most iterations using ordinary 64-bit IEEE arithmetic, are described in [23].

High-precision arithmetic must be used for almost all applications of integer relation detection methods, using PSLQ or any other algorithm. This stems from the fact that if one wishes to recover a relation of length n, with coefficients of maximum size d digits, then the input vector x must be specified to at least nd digits, and one must employ floating-point arithmetic accurate to at least nd digits, or else the true solution will be lost in a sea of numerical artifacts. PSLQ typically recovers relations when the input data is specified to at least 10% or 15% greater precision than this minimum value, and when a working precision of at least this level is used to implement PSLQ.

PSLQ operates by constructing a series of matrices A_k, such that the entries of the vector $y_k = A_k^{-1}x$ steadily decrease in size. At any given iteration, the largest and smallest entries of y_k usually normally differ by no more than two or three

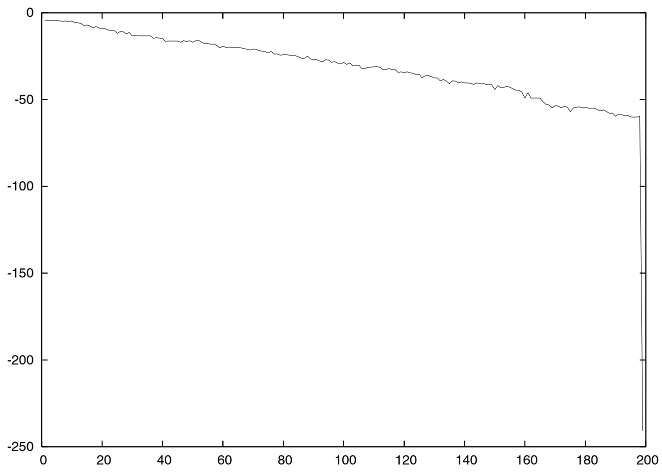


Figure 2.1. Plot of $\log_{10}(\min_i |x_i|)$ in a typical PSLQ run as a function of the iteration number.

orders of magnitude. When a relation is detected by the algorithm, the smallest entry of the y_k vector abruptly decreases to roughly the epsilon of the working precision (i.e., 10^{-p}, where p is the precision level in digits), and the desired relation is given by the corresponding column of A_k^{-1}. See Figure 2.1, which shows this behavior for a typical PSLQ computation (see Section 8.8).

The detection threshold in the termination test for PSLQ is typically set to be a few orders of magnitude greater than the epsilon value in order to allow for reliable relation detection in the presence of some numerical roundoff error. The ratio between the smallest and the largest entry of the vector $A^{-1}x$ when a relation is detected can be taken as a "confidence level" that the relation is a true relation and not an artifact of insufficient numeric precision. Very small ratios at detection, such as 10^{-100}, almost certainly denote a true relation (although, of course, such results are experimental only, and do not constitute rigorous proof).

2.4 Illustrations and Examples

2.4.1 The BBP Formula for Pi

Perhaps the best-known application of PSLQ is the 1995 discovery, by means of a PSLQ computation, of the BBP formula for π,

$$\pi = \sum_{k=0}^{\infty} \frac{1}{16^k}\left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6}\right). \tag{2.1}$$

This formula permits one to directly calculate binary or hexadecimal digits beginning at the nth digit, without the need to calculate any of the first $n-1$ digits, using a simple algorithm and standard 64-bit or 128-bit arithmetic [22].

The genesis of this discovery was the realization, by Peter Borwein and Simon Plouffe, that individual binary digits of log2 could be calculated, by applying the well-known classical formula

$$\log 2 = \sum_{k=1}^{\infty} \frac{1}{k2^k}. \tag{2.2}$$

Suppose that 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

$$\begin{aligned} \{2^d \log 2\} &= \left\{\left\{\sum_{k=0}^{d} \frac{2^{d-k}}{k}\right\} + \sum_{k=d+1}^{\infty} \frac{2^{d-k}}{k}\right\} \\ &= \left\{\left\{\sum_{k=0}^{d} \frac{2^{d-k} \bmod k}{k}\right\} + \sum_{k=d+1}^{\infty} \frac{2^{d-k}}{k}\right\}. \end{aligned} \tag{2.3}$$

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 (2.3), 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 $3^{17} = ((((3^2)^2)^2)^2) \cdot 3 = 129,140,163$, thus producing the result in only 5 multiplications, instead of the usual 16. If we are only interested in the result modulo 10, then we can calculate $((((3^2 \bmod 10)^2 \bmod 10)^2 \bmod 10)^2 \bmod 10) \cdot 3 \bmod 10 = 3$, and we never have to store or operate on integers larger than 81. Indeed, this particular calculation can be done in one's head.

Since we can very rapidly evaluate each term of the first summation in (2.3), and since the second summation can be truncated after just a few terms, it is clear one can quickly calculate, say, the first 40 digits of the binary expansion of log2, beginning with some position $d+1$, where $d < 10^7$, using only standard IEEE 64-bit floating-point arithmetic. If one uses 128-bit floating-point arithmetic, or "double-double" arithmetic, then one can calculate more digits beginning at the desired position $d+1$, and this calculation is reliable for $d \leq 10^{15}$.

After this discovery by Peter Borwein and Simon Plouffe, they immediately began to investigate whether individual digits of π could be computed in this manner. It is clear that we can employ this technique on any constant that can be written using a formula of the form

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

where $b > 1$ is an integer and p and q are polynomials with integer coefficients, with q having no zeroes at positive integer arguments. However, at this time (1995), there were no known formulas for π of this form. So they began to investigate (with the help of Bailey's PSLQ computer program) whether π was a linear combination of other constants that are of this form. These computer runs were redone numerous times over the course of two or three months, as new constants of the requisite form were found in the literature. Eventually, the BBP formula for π was discovered.

Table 2.1 gives some results of calculations that have been done in this manner. The last-listed result, which is tantamount to a computation of the one-quadrillionth binary digit of π, was performed on over 1,700 computers worldwide, using software written by Colin Percival.

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 2.1. Computed hexadecimal digits of π.

The BBP formula for π has even found a practical application—it is now used in the g95 Fortran compiler as part of the procedure for evaluating certain transcendental functions.

2.4.2 Bifurcation Points in Chaos Theory

One application of integer relation detection methods is to find the minimal polynomial of an algebraic constant. Note that if α satisfies a polynomial $a_0 + a_1 t + \cdots + a_n = 0$, then we can discover this polynomial simply by computing, to high precision, the values of $1, \alpha, \alpha^2, \cdots, \alpha^n$, and then applying PSLQ or some other integer relation scheme to the resulting $(n+1)$-long vector.

The chaotic iteration $x_{k+1} = rx_k(1-x_k)$ has been studied since the early days of chaos theory in the 1950s. It is often called the "logistic iteration," since it mimics the behavior of an ecological population that, if its growth one year outstrips its food supply, often falls back in numbers for the following year, thus continuing to vary in a highly irregular fashion. When r is less than one, iterates of the logistic iteration converge to zero. For r in the range $1 < r < B_1 = 3$, iterates converge to some nonzero limit. If $B_1 < r < B_2 = 1 + \sqrt{6} = 3.449489\ldots$, the limiting behavior bifurcates—every other iterate converges to a distinct limit point. For r with $B_2 < r < B_3$, iterates select between a set of four distinct limit points; when $B_3 < r < B_4$, they select between a set of eight distinct limit points; this pattern repeats until $r > B_\infty = 3.569945672\ldots$, when the iteration is completely chaotic (see Figure 2.2). The limiting ratio $\lim_N (B_N - B_{N-1})/(B_{N+1} - B_N) = 4.669201\ldots$ is known as *Feigenbaum's delta constant*.

It is fairly easy to see that all of these B constants are algebraic numbers, but the bounds one obtains on the degree are often rather large, and thus not very useful. Thus one may consider using PSLQ or some other integer relation algorithm to discover their minimal polynomials.

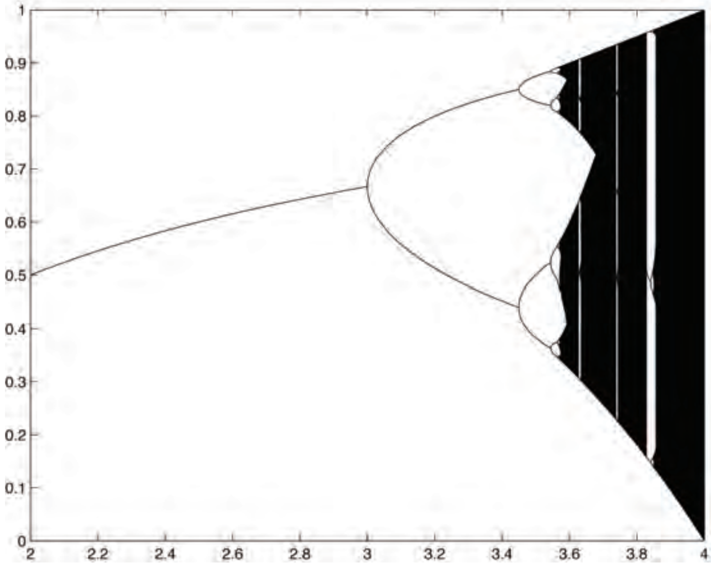


Figure 2.2. Bifurcation in the logistic iteration.

A highly accurate numerical value of B_3, for instance, can be obtained using a relatively straightforward search scheme. Let $f_8(r,x)$ be the eight-times iterated evaluation of $rx(1-x)$, and let $g_8(r,x) = f_8(r,x) - x$. Imagine a three-dimensional graph, where r ranges from left to right and x ranges from bottom to top (as in Figure 2.2), and where $g_8(r,x)$ is plotted in the vertical (out-of-plane) dimension. Given some initial r slightly less than B_3, we compute a "comb" of function values at m evenly spaced x values (with spacing h_x) near the limit of the iteration $x_{k+1} = f_8(r,x_k)$. In our implementation, we use $m = 12$, and we start with $r = 3.544, x = 0.364, h_r = 10^{-4}$, and $h_x = 5 \times 10^{-4}$. With this construction, the "comb" has $m/2$ negative function values, followed by $m/2$ positive function values. We then increment r by h_r and re-evaluate the "comb," continuing in this fashion until two sign changes are observed among the m function values of the "comb." This means that a bifurcation occurred just prior to the current value of r, so we restore r to its previous value (by subtracting h_r), reduce h_r, say by a factor of four, and also reduce the h_x roughly by a factor of 2.5. We continue in this fashion, moving the value of r and its associated "comb" back and forth near the bifurcation point with progressively smaller intervals h_r. The center of the "comb" in the x direction must be adjusted periodically to ensure that $m/2$ negative function values are followed by $m/2$ positive function values, and the spacing parameter h_x must be adjusted as well to ensure that two sign changes are disclosed when this occurs. We quit when the smallest of the m function values is within two or three orders of magnitude of the epsilon of the arithmetic (e.g., for 2000-digit working precision, epsilon is 10^{-2000}). The final value of r is then the desired value B_3, accurate to within a tolerance given by the final value of r_h. With 2000-digit working precision, our implementation of this scheme finds B_3 to 1330-digit accuracy in about five minutes on a 2004-era computer. The first hundred digits are as follows:

$$\begin{aligned} B_3 \;=\; & 3.54409035955192285361596598660480454058309984544457 \\ & 36754578125303058429428588630122562585664248917999 6 \\ & 26\ldots \end{aligned}$$

With even a moderately accurate value of r in hand (at least two hundred digits or so), one can use a PSLQ program to check to see whether r is an algebraic constant. When $n \geq 12$, the relation

$$\begin{aligned} 0 = r^{12} - 12r^{11} + 48r^{10} - 40r^9 - 193r^8 + 392r^7 + 44r^6 + 8r^5 - 977r^4 \\ - 604r^3 + 2108r^2 + 4913 \end{aligned} \tag{2.4}$$

can be recovered.

The significantly more challenging problem of computing and analyzing the constant $B_4 = 3.564407266095\ldots$ is discussed in [23]. In this study, conjectural reasoning suggested that B_4 might satisfy a 240-degree polynomial, and, in addition, that $\alpha = -B_4(B_4 - 2)$ might satisfy a 120-degree polynomial. The constant α was then computed to over 10,000-digit accuracy, and an advanced three-level, multi-pair PSLQ program was employed, running on a parallel computer system, to find an integer relation for the vector $(1, \alpha, \alpha^2, \cdots, \alpha^{120})$. A numerically significant solution was obtained, with integer coefficients descending monotonically from 257^{30}, which is a 73-digit integer, to the final value, which is 1 (a striking result that is exceedingly unlikely to be a numerical artifact). This experimentally discovered polynomial was recently confirmed in a large symbolic computation [186].

Additional information on the Logistic Map is available at http://mathworld.wolfram.com/LogisticMap.html [278].

2.4.3 Sculpture

The PSLQ algorithm was discovered in 1993 by Helaman Ferguson. This is certainly a signal accomplishment—as already mentioned, the PSLQ algorithm (with associated lattice reduction algorithms) was recently named one of ten "algorithms of the century" by *Computing in Science and Engineering* [10]. 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 [134]. Together, the Fergusons recently won the 2002 Communications Award, bestowed by the Joint Policy Board of Mathematics.

Ferguson notes that the PSLQ algorithm can be thought of as an *n*-dimension extension of the Euclidean algorithm, and is, like the Euclidean scheme, fundamentally a subtractive algorithm. As Ferguson explains, "It is also true that my sculptural form of expression is subtractive: I get my mathematical forms by direct carving of stone" [239].

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

One of Ferguson's well-known sculptures is the *Figure-Eight Complement II* (see Figure 2.3). It has been known for some time that the hyperbolic volume V of the figure-eight knot complement is given by the formula

$$
\begin{aligned}
V &= 2\sqrt{3}\sum_{n=1}^{\infty}\frac{1}{n\binom{2n}{n}}\sum_{k=n}^{2n-1}\frac{1}{k} \\
&= 2.02988321281930725004240510854 9\ldots.
\end{aligned}
\tag{2.5}
$$

Figure 2.3. Ferguson's *Figure-Eight Knot Complement II* sculpture.

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

$$C_j \quad = \quad \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n(6n+j)^2}. \qquad (2.6)$$

Indeed, it is, as Broadhurst [75] found using a PSLQ program,

$$V \quad = \quad \frac{\sqrt{3}}{9} \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n} \left[\frac{18}{(6n+1)^2} - \frac{18}{(6n+2)^2} - \frac{24}{(6n+3)^2} - \frac{6}{(6n+4)^2} + \frac{2}{(6n+5)^2} \right]. \qquad (2.7)$$

You can verify this yourself, using for example the Mathematician's Toolkit, available at [15] http://www.experimentalmath.info. Just type the following lines of code in *Mathematica*:

```
v = 2 * sqrt[3]
* sum[1/(n * binomial[2*n,n]) * sum[1/k, \
  {k, n, 2*n-1}], {n, 1, infinity}]
pslq[v/sqrt[3], table[sum[(-1)^n/(27^n*(6*n+j)^2), \
  {n, 0, infinity}], {j, 1, 6}]]
```

When this is done, you will recover the solution vector $(9,-18,18,24,6,-2,0)$. A proof that formula (2.7) holds, together with a number of other identities for V, is given in [50, pp. 88–92]. This proof, by the way, is a classic example of experimental methodology, in that it relies on knowing ahead of time that the formula holds.

2.4.4 Euler Sums

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

$$\sum_{k=1}^{\infty} \left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^2 k^{-2} \quad = \quad 4.59987\ldots \quad \approx \quad \frac{17}{4}\zeta(4) \quad = \quad \frac{17\pi^4}{360}. \qquad (2.8)$$

The function $\zeta(s)$ in (2.8) is the classical *Riemann zeta function*

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

Au-Yeung had computed the sum in (2.8) to 500,000 terms, giving an accuracy of five or six decimal digits. Suspecting that his discovery was merely a modest numerical coincidence, Borwein sought to compute the sum to a higher level of precision. Using Fourier analysis and Parseval's equation, he obtained

$$\frac{1}{2\pi}\int_0^\pi (\pi-t)^2\log^2(2\sin\frac{t}{2})\,dt \quad = \quad \sum_{k=1}^\infty \left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^2 (k+1)^{-2}. \tag{2.9}$$

The series on the right of (2.9) permits one to evaluate (2.8), while the integral on the left can be computed using the numerical quadrature facility of *Mathematica* or *Maple*. When he did this, Borwein was surprised to find that the conjectured identity holds to more than thirty digits.

The summation in (2.9) can be reduced to a combination of *multivariate zeta values*, which in general are defined as

$$\zeta(s_1,s_2,\cdots,s_m) \quad = \quad \sum_{n_1>n_2>\cdots>n_m>0}\prod_{j=1}^m n_j^{-|s_j|}\sigma_j^{-n_j},$$

where the $s_1,s_2,\ldots,s_m$ are nonzero integers and $\sigma_j = \mathrm{signum}(s_j)$. (We have already seen an example in Section 1.6.) A fast method for computing such sums, based on Hölder convolution, is discussed in [58] and is also discussed in Section 2.6 below. For the time being, it suffices to note that the scheme is implemented in EZFace+, an online tool available at [83] http://oldweb.cecm.sfu.ca/projects/ezface+. We will illustrate its application to one specific case, namely the analytic identification of the sum

$$S_{2,3} \quad = \quad \sum_{k=1}^\infty \left(1-\frac{1}{2}+\cdots+(-1)^{k+1}\frac{1}{k}\right)^2 \frac{1}{(k+1)^3}. \tag{2.10}$$

Expanding the squared term in (2.10), we have

$$S_{2,3} \quad = \quad \sum_{0<i,j<k}\frac{(-1)^{i+j}}{ijk^3} \;=\; 2\,\zeta(3,-1,-1)+\zeta(3,2). \tag{2.11}$$

Evaluating this in EZFace+, we quickly obtain

$$\begin{aligned}S_{2,3} = 0.&15616693338117691588103590968798819368577670984\,03\\ &03872957529354497075037440295791455205653709358\,1475\\ &78\ldots.\end{aligned}$$

Based on our experience with other multivariate zeta values, we conjectured that this constant satisfies a rational linear relation involving the following constants: π^5, $\pi^4\log(2)$, $\pi^3\log^2(2)$, $\pi^2\log^3(2)$, $\pi\log^4(2)$, $\log^5(2)$, $\pi^2\zeta(3)$, $\pi\log(2)\zeta(3)$, $\log^2(2)\zeta(3)$, $\zeta(5)$, and $\mathrm{Li}_5(1/2)$, where

$$\mathrm{Li}_n(x) := \sum_{k>0} x^k/k^n \tag{2.12}$$

denotes the polylogarithm function. Note that each of these constants can be seen to have "degree" five. The result is quickly found to be

$$S_{2,3} = 4\,\mathrm{Li}_5\left(\frac{1}{2}\right) - \frac{1}{30}\log^5(2) - \frac{17}{32}\zeta(5) - \frac{11}{720}\pi^4\log(2) + \frac{7}{4}\zeta(3)\log^2(2) + \frac{1}{18}\pi^2\log^3(2) - \frac{1}{8}\pi^2\zeta(3).$$

This result has been proved in various ways, both analytic and algebraic. Indeed, all evaluations of sums of the form $\zeta(\pm a_1, \pm a_2, \cdots, \pm a_m)$ with *weight* $w := \sum_j a_j < 8$, as in (2.11), have been established.

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, rigorously established results [47]. A few examples include

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

$$\sum_{n=1}^{\infty}\left(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{n}\right)^4\frac{1}{(n+1)^5} = -\frac{29}{2}\zeta(9) + \frac{37}{2}\zeta(4)\zeta(5) + \frac{33}{4}\zeta(3)\zeta(6) - \frac{8}{3}\zeta^3(3) - 7\zeta(2)\zeta(7),$$

$$\sum_{k=1}^{\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^3\frac{1}{(k+1)^6} = \zeta^3(3) + \frac{197}{24}\zeta(9) + \frac{1}{2}\pi^2\zeta(7) - \frac{11}{120}\pi^4\zeta(5) - \frac{37}{7560}\pi^6\zeta(3). \tag{2.13}$$

2.4.5 Quantum Field Theory

In another recent development, David Broadhurst (who discovered the identity (2.7) 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 [76, 77]. In particular, the renormalization procedure (which removes infinities from the perturbation expansion) involves multivariate zeta values. He has shown [75], 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

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

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 2.4. 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 2.2. In the table the constant $C = \sum_{k>0}\sin(\pi k/3)/k^2$.

Some additional details for the examples in this section are available in [50, Chapter 2] and [21].

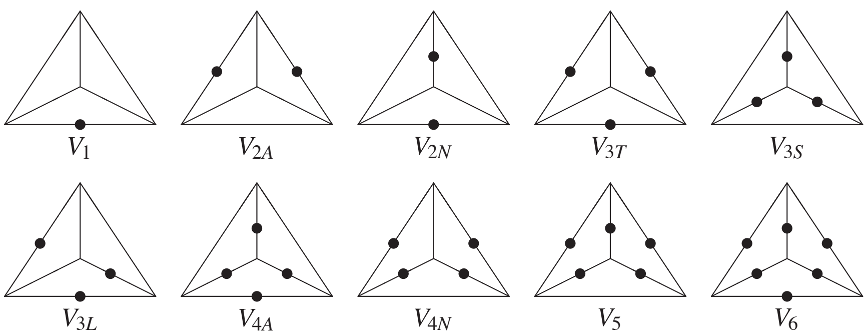


Figure 2.4. The ten tetrahedral configurations.

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	$=$	$6\zeta(3)-13\zeta(4)-8U-4C^2$

Table 2.2. Formulas found by PSLQ for the ten tetrahedral diagrams.

2.5 Definite Integrals and Infinite Series Summations

One particularly useful application of integer relation computations is to evaluate definite integrals and sums of infinite series by means of numerical calculations. We use one of various methods to obtain a numerical value for the integral or summation, then try to identify this value by means of integer relation methods.

In many cases, one can apply online tools (which employ integer relation techniques combined with large-scale table-lookup schemes) to blindly identify numerical values. One of the most popular and effective tools is the already mentioned Inverse Symbolic Calculator (ISC) tool, available at [84] http://oldweb.cecm.sfu.ca/projects/ISC.

In other cases, these tools are unable to identify the constant, and custom-written programs must be used, which typically take advantage of knowledge that certain sums are likely to involve a certain class of constants.

As one example, we were inspired by a recent problem in the *American Mathematical Monthly* [3]. By using one of the quadrature routines to be described in the next section, together with the ISC tool and a PSLQ integer relation detection program, we found that if $C(a)$ is defined by

$$C(a) \quad = \quad \int_0^1 \frac{\arctan(\sqrt{x^2+a^2})\,dx}{\sqrt{x^2+a^2}(x^2+1)}, \tag{2.14}$$

then

$$C(0) \quad = \quad \pi \log 2/8 + G/2,$$

$$\begin{aligned} C(1) &= \pi/4 - \pi\sqrt{2}/2 + 3\sqrt{2}\arctan(\sqrt{2})/2, \\ C(\sqrt{2}) &= 5\pi^2/96, \end{aligned} \tag{2.15}$$

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:

$$\begin{aligned} &\int_0^\infty \frac{\arctan(\sqrt{x^2+a^2})\,dx}{\sqrt{x^2+a^2}(x^2+1)} \\ &= \frac{\pi}{2\sqrt{a^2-1}}\left[2\arctan(\sqrt{a^2-1}) - \arctan(\sqrt{a^4-1})\right]. \end{aligned} \tag{2.16}$$

We will discuss techniques for computing definite integrals and sums of series to high precision in Chapter 3. 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.

2.6 Computation of Multivariate Zeta Values

One class of mathematical constants that has been of particular interest to experimental mathematicians in the past few years is multivariate zeta values (which we have already seen in Example 1.5 and in Section 2.4.4 above). Research in this arena has been facilitated by the discovery of methods that permit the computation of these constants to high precision. While Euler-Maclaurin-based schemes can be used (and in fact were used) in these studies, they are limited to 2-order sums. We present here an algorithm that permits even high-order sums to be evaluated to hundreds or thousands of digit accuracy. We will limit our discussion here to multivariate zeta values of the form

$$\zeta(s_1, s_2, \cdots, s_k) = \sum_{n_1 > n_2 > \cdots > n_k} \frac{1}{n_1^{s_1} n_2^{s_2} \cdots n_k^{s_k}} \tag{2.17}$$

for positive integers s_j and n_j, i.e., to Euler sums, although in general the technique we describe here has somewhat broader applicability.

This scheme is as follows [58]. For $1 \leq j \leq m$, define the numeric strings

$$a_j = \{s_j + 2, \{1\}_{r_j}, s_{j+1}, \{1\}_{r_{j+1}}, \cdots, s_m + 2, \{1\}_{r_m}\}, \tag{2.18}$$

$$b_j = \{r_j + 2, \{1\}_{s_j}, r_{j-1}, \{1\}_{s_{j-1}}, \cdots, r_1 + 2, \{1\}_{s_1}\}, \tag{2.19}$$

for any nonnegative integers r_n, s_n, where by the notation $\{1\}_n$ we mean n repetitions of 1, as before. For convenience, we will define a_{m+1} and b_0 to be the empty string.

Define

$$\kappa(s_1, s_2, \cdots, s_k) = \sum_{n_j > n_{j+1} > 0} 2^{-n_1} \prod_{j=1}^{k} n_j^{-s_j}. \tag{2.20}$$

Then we have the so-called *Hölder convolution*

$$\begin{aligned} \zeta(a_1) = & \sum_{j=1}^{m} \left[\sum_{t=0}^{s_j+1} \kappa(s_j + 2 - t, \{1\}_{r_j}, a_{j+1}) \kappa(\{1\}_t, b_{j-1}) \right. \\ & \left. + \sum_{u=1}^{r_j} \kappa(\{1\}_u, a_{j+1}) \kappa(r_j + 2 - u, 1_{s_j}, b_{j-1}) \right] + \kappa(b_m). \end{aligned} \tag{2.21}$$

See the discussion in Chapter 3 of [51] for further details. As mentioned above, EZFace+ [83] implements this procedure. The procedure has also been implemented as part of the Experimental Mathematician's Toolkit [15], available at http://www.experimentalmath.info.

2.7 Ramanujan-Type Elliptic Series

Truly new types of infinite series formulas, based on elliptic integral approximations, were discovered by Srinivasa Ramanujan (1887–1920) around 1910, but were not well known (nor fully proven) until quite recently when his writings were widely published. They are based on elliptic functions and are described at length in [52]. One of these is the remarkable formula

$$\frac{1}{\pi} = \frac{2\sqrt{2}}{9801} \sum_{k=0}^{\infty} \frac{(4k)!\,(1103 + 26390k)}{(k!)^4 396^{4k}}. \tag{2.22}$$

Each term of this series produces an additional *eight* correct digits in the result. When Gosper used this formula to compute 17 million digits of π in 1985, and it agreed to many millions of places with the prior estimates, *this concluded the first proof* of (2.22), as described in [52]. Actually, Gosper first computed the simple continued fraction for π, hoping to discover some new things in its expansion, but found none. At about the same time, David and Gregory Chudnovsky found the following rational variation of Ramanujan's formula. It exists because $\sqrt{-163}$ corresponds to an imaginary quadratic field with class number one:

$$\frac{1}{\pi} = 12 \sum_{k=0}^{\infty} \frac{(-1)^k\,(6k)!\,(13591409 + 545140134k)}{(3k)!\,(k!)^3\,640320^{3k+3/2}}. \tag{2.23}$$

Each term of this series produces an additional 14 correct digits. The Chudnovskys implemented this formula using a clever scheme that enabled them to use the results of an initial level of precision to extend the calculation to even higher precision. They used this in several large calculations of π, culminating with a *record computation* (in 1994) to over four billion decimal digits. Their remarkable story was compellingly told by Richard Preston in a prizewinning *New Yorker* article "The Mountains of Pi" [238].

While these Ramanujan and Chudnovsky series are in practice considerably more efficient than classical formulas, they share the property that the number of terms needed increases linearly with the number of digits desired: *If you wish to compute twice as many digits of π, you must evaluate twice as many terms of the series.* Relatedly, the Ramanujan-type series

$$\frac{1}{\pi} = \sum_{n=0}^{\infty} \left(\frac{\binom{2n}{n}}{16^n} \right)^3 \frac{42n+5}{16} \tag{2.24}$$

allows one to compute the billionth binary digit of $1/\pi$, or the like, *without computing the first half* of the series.

In some recent papers, J. Guillera has exhibited several new Ramanujan-style series formulas for reciprocal powers of π, including the following [154–156]:

$$\frac{128}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (13 + 180n + 820n^2) \left(\frac{1}{32}\right)^{2n}, \tag{2.25}$$

$$\frac{32}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (1 + 8n + 20n^2) \left(\frac{1}{2}\right)^{2n}, \tag{2.26}$$

$$\frac{32}{\pi^3} = \sum_{n=0}^{\infty} r(n)^7 (1 + 14n + 76n^2 + 168n^3) \left(\frac{1}{32}\right)^{2n}, \tag{2.27}$$

where we define the function $r(n)$ as

$$r(n) = \frac{(1/2)_n}{n!} = \frac{1/2 \cdot 3/2 \cdot \cdots \cdot (2n-1)/2}{n!} = \frac{\Gamma(n+1/2)}{\sqrt{\pi}\,\Gamma(n+1)}.$$

Guillera proved (2.25) and (2.26) using Wilf-Zeilberger's method described in Chapter 3. He ascribes series (2.27) to Gourevich who also found it using integer relation methods. Guillera also provides other series for $1/\pi^2$ based on other Gamma function values as in (2.22) and (2.23), but for our experiments we restrict ourselves to $r(n)$.

2.7.1 Experiments with Ramanujan-Type Series

We have attempted to do a more thorough experimental search for identities of this general type. In particular, we searched for formulas of either of the two forms

$$\frac{c}{\pi^m} = \sum_{n=0}^{\infty} r(n)^{2m+1}(p_0 + p_1 n + \cdots + p_m n^m)\alpha^{2n}, \tag{2.28}$$

$$\frac{c}{\pi^m} = \sum_{n=0}^{\infty} (-1)^n r(n)^{2m+1}(p_0 + p_1 n + \cdots + p_m n^m)\alpha^{2n}. \tag{2.29}$$

Here c is some integer linear combination of the constants $(d_i,\ 1 \le i \le 34)$

$$1, 2^{1/2}, 2^{1/3}, 2^{1/4}, 2^{1/6}, 4^{1/3}, 8^{1/4}, 32^{1/6}, 3^{1/2}, 3^{1/3}, 3^{1/4}, 3^{1/6}, 9^{1/3},$$
$$27^{1/4}, 243^{1/6}, 5^{1/2}, 5^{1/4}, 125^{1/4}, 7^{1/2}, 13^{1/2}, 6^{1/2}, 6^{1/3}, 6^{1/4}, 6^{1/6},$$
$$7, 36^{1/3}, 216^{1/4}, 7776^{1/6}, 12^{1/4}, 108^{1/4}, 10^{1/2}, 10^{1/4}, 15^{1/2}.$$

The polynomial coefficients $(p_k,\ 1 \le k \le m)$ in (2.28) and (2.29) are each some integer linear combination of the constants $(q_i,\ 1 \le i \le 11)$

$$1, 2^{1/2}, 3^{1/2}, 5^{1/2}, 6^{1/2}, 7^{1/2}, 10^{1/2}, 13^{1/2}, 14^{1/2}, 15^{1/2}, 30^{1/2}.$$

Note that the linear combination chosen for a given p_k may be different from that chosen for any of the others. The constant α in (2.28) and (2.29) is chosen from

$$1/2,\ 1/4,\ 1/8,\ 1/16,\ 1/32,\ 1/64,\ 1/128,\ 1/256,\ \sqrt{5}-2,\ (2-\sqrt{3})^2,$$
$$5\sqrt{13}-18,\ (\sqrt{5}-1)^4/128,\ (\sqrt{5}-2)^4,\ (2^{1/3}-1)^4/2,\ 1/(2\sqrt{2}),$$
$$(\sqrt{2}-1)^2,\ (\sqrt{5}-2)^2,\ (\sqrt{3}-\sqrt{2})^4.$$

This list of α constants was taken from a table on page 172 of [52].

These searches were done using a two-level PSLQ integer relation finding program, with 1000-digit precision. Each selection of m and α constituted one separate integer relation search. In particular, for a fixed m and α in (2.28), we calculated the $[34 + 11(m+1)]$-long set of real numbers

$$d_1, d_2, \cdots, d_{34}, \tag{2.30}$$

$$q_0 \sum_{n=0}^{\infty} r(n)^{2m+1}\alpha^{2n}, q_1 \sum_{n=0}^{\infty} r(n)^{2m+1}\alpha^{2n}, \cdots, q_{11} \sum_{n=0}^{\infty} r(n)^{2m+1}\alpha^{2n}, \tag{2.31}$$

$$q_1 \sum_{n=0}^{\infty} r(n)^{2m+1} n\alpha^{2n}, q_2 \sum_{n=0}^{\infty} r(n)^{2m+1} n\alpha^{2n}, \cdots, q_{11} \sum_{n=0}^{\infty} r(n)^{2m+1} n\alpha^{2n}, \cdots, \tag{2.32}$$

$$q_1 \sum_{n=0}^{\infty} r(n)^{2m+1} n^m\alpha^{2n}, q_2 \sum_{n=0}^{\infty} r(n)^{2m+1} n^m\alpha^{2n}, \cdots, q_{11} \sum_{n=0}^{\infty} r(n)^{2m+1} n^m\alpha^{2n} \tag{2.33}$$

and then applied a two-level PSLQ program, implemented using ARPREC multiple-precision software, to this vector.

After finding a relation with our program, we carefully checked to ensure that it was not reducible to another in the list by an algebraic manipulation. Also, in numerous cases, multiple relations existed. In such cases, we eliminated these one by one, typically by replacing one of the constants in the relation by an unrelated transcendental and re-running the program, until no additional relations were found.

The result of this effort is the following list of relations. As it turns out, each of these is given either implicitly or explicitly in [52] or [155]. But just as important here is the apparent nonexistence of additional relations. In particular, if a relation is not shown below for a given α and/or sign choice, that means (as a consequence of our calculations) that there is no such relation with integer coefficients whose Euclidean norm is less than 10^{10}.

For degree $m = 1$, with nonalternating signs,

$$\frac{4}{\pi} = \sum_{n=0}^{\infty} r(n)^3 (1+6n) \left(\frac{1}{2}\right)^{2n},$$

$$\frac{16}{\pi} = \sum_{n=0}^{\infty} r(n)^3 (5+42n) \left(\frac{1}{8}\right)^{2n},$$

$$\frac{12^{1/4}}{\pi} = \sum_{n=0}^{\infty} r(n)^3 (-15+9\sqrt{3}-36n+24\sqrt{3}n) \left(2-\sqrt{3}\right)^{4n},$$

$$\frac{32}{\pi} = \sum_{n=0}^{\infty} r(n)^3 (-1+5\sqrt{5}+30n+42\sqrt{5}n) \left(\frac{(\sqrt{5}-1)^4}{128}\right)^{2n},$$

$$\frac{5^{1/4}}{\pi} = \sum_{n=0}^{\infty} r(n)^3 (-525+235\sqrt{5}-1200n+540\sqrt{5}n) \left(\sqrt{5}-2\right)^{8n}.$$

For degree $m = 1$, with alternating signs,

$$\frac{2\sqrt{2}}{\pi} = \sum_{n=0}^{\infty} (-1)^n r(n)^3 (1+6n) \left(\frac{1}{2\sqrt{2}}\right)^{2n},$$

$$\frac{2}{\pi} = \sum_{n=0}^{\infty} (-1)^n r(n)^3 (-5+4\sqrt{2}-12n+12\sqrt{2}n) \left(\sqrt{2}-1\right)^{4n},$$

$$\frac{2}{\pi} = \sum_{n=0}^{\infty} (-1)^n r(n)^3 (23-10\sqrt{5}+60n-24\sqrt{5}n) \left(\sqrt{5}-2\right)^{4n},$$

$$\frac{2}{\pi} = \sum_{n=0}^{\infty} (-1)^n r(n)^3 (177-72\sqrt{6}+420n-168\sqrt{6}n) \left(\sqrt{3}-\sqrt{2}\right)^{8n}.$$

For degree $m = 2$,

$$\frac{8}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (1+8n+20n^2) \left(\frac{1}{2}\right)^{2n},$$

$$\frac{128}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (13+180n+820n^2) \left(\frac{1}{32}\right)^{2n}.$$

For degree $m = 3$,

$$\frac{32}{\pi^3} = \sum_{n=0}^{\infty} r(n)^7 (1+14n+76n^2+168n^3) \left(\frac{1}{8}\right)^{2n}.$$

For degree $m = 4,5$ we have been unable to find any similar series, with exclusion bounds roughly 10^{10} as before, thereby (so far) dashing our hope to find an infinite family of rational sums extending (2.24), (2.25), (2.26), and (2.27). More study, however, will be needed to understand this phenomenon.

2.7.2 Working with the Series Analytically

While (2.25), (2.26), and (2.27) have no explanation, there are tantalizing echoes of the elliptic theory described in [52] that explains the series for $1/\pi$ as we now partially reprise. We first define the *theta functions* θ_3, θ_4, and θ_2 as

$$\theta_2(q) := \sum_{n=-\infty}^{\infty} q^{(n+1/2)^2}, \quad \theta_3(q) := \sum_{n=-\infty}^{\infty} q^{n^2}, \quad \theta_4(q) := \sum_{n=-\infty}^{\infty} (-1)^n q^{n^2},$$

for $|q| < 1$. We next identify the *invariant*

$$k_N = \frac{\theta_2^2}{\theta_3^2}\left(e^{-\pi\sqrt{N}}\right).$$

We denote the *complementary modulus* $k' := \sqrt{1-k^2}$ in terms of which it transpires that Jacobi's identity $\theta_3^4 = \theta_4^4 + \theta_2^4$ (see [52]) implies

$$k_N^{'} = \frac{\theta_4^2}{\theta_3^2}\left(e^{-\pi\sqrt{N}}\right).$$

For reasons detailed in [51] and [52], we know that, for each natural number N, k_N is algebraic.

For example, $k_1 = 1/\sqrt{2} = k_1'$ while k_{210} is the *singular value* sent to Hardy in Ramanujan's famous 1913 letters of introduction—ignored by two other famous English mathematicians:

$$\begin{aligned} k_{210} := {} & \left(\sqrt{2}-1\right)^2 \left(\sqrt{3}-2\right) \left(\sqrt{7}-6\right)^2 \left(8-3\sqrt{7}\right) \\ & \times \left(\sqrt{10}-3\right)^2 \left(\sqrt{15}-\sqrt{14}\right) \left(4-\sqrt{15}\right)^2 \left(6-\sqrt{35}\right). \end{aligned}$$

Remarkably,

$$k_{100} \quad := \quad \left(\left(3-2\sqrt{2}\right)\left(2+\sqrt{5}\right)\left(-3+\sqrt{10}\right)\left(-\sqrt{2}+\sqrt[4]{5}\right)^2\right)^2$$

arose in Bornemann's solution to Trefethen's tenth problem [275]: The probability that a Brownian motion starting at the center of a 10×1 box hits the ends first is $2/\pi \arcsin(k_{100})$. Ramanujan also noticed that the invariants G_N and g_N defined next are often simpler:

$$G_N^{-12} := 2k_N k_N' \text{ and } g_N^{-12} := 2k_N/k_N'^2.$$

Note that each of these two latter invariants provides a quadratic formula for k_N. We also need *Ramanujan's invariant of the second kind*

$$\alpha_N := \frac{1/\pi - q\theta_4'(q)/\theta_4(q)}{\theta_3^4(q)}, \qquad q := e^{-\pi\sqrt{N}}, \tag{2.34}$$

which is also algebraic for integer N [52]. In the form we have given them all the coefficients are very simple to compute numerically. Hence integer relation methods are easy to apply.

Example 2.1 (Determining Invariants). The following *Maple* code produces 20 digits of each of our invariants:

```
que:=N->exp(-Pi*sqrt(N)):
kk:=q->(JacobiTheta2(0,q)/JacobiTheta3(0,q))^2:
kc:=q->(JacobiTheta4(0,q)/JacobiTheta3(0,q))^2: k:=kk@que:
l:=kc@que: G:=1/(2*k*l): g:=2*k/l^2:
alpha:=r->(subs(q=exp(-Pi*sqrt(r)),
  (1/Pi-sqrt(r)*4*(q*diff(JacobiTheta4(0,q),q)/
  JacobiTheta4(0,q)))/JacobiTheta3(0,q)^4)):
  a0:=N->(alpha(N)-sqrt(N)*k(N)^2):
  a1:=N->sqrt(N)*(1-2*k(N)^2):
  b0:=N->alpha(N)/(1-k(N)^2):
  b1:=N->sqrt(N)*(1+k(N)^2)/(1-k(N)^2):
```

◇

We first explore use of *Maple*'s `identify` function. Entering

```
for n to 6 do identify(evalf[20](k(n))) od;
```

returns

$$1/2\sqrt{2},\ -1+\sqrt{2},\ 1/4\sqrt{6}-1/4\sqrt{2},\ 3-2\sqrt{2},$$

$$0.11887694580260010118,\ 0.085164233174742587643,$$

where we have used only the simplest parameter-free version of the `identify` function. Correspondingly,

```
for n to 8 do identify(evalf[20](G(2*n-1))) od;
```

returns

$$1,\,2,\,2+\sqrt{5},\,87+4\sqrt{3},\,4/3\sqrt[3]{199+3\sqrt{33}}+\frac{136}{3}\frac{1}{\sqrt[3]{199+3\sqrt{33}}}+\frac{22}{3},$$

$$18+5\sqrt{13},\,28+12\sqrt{5},$$

for the first seven odd values of G_N^{-12}, and

```
for n to 8 do identify(evalf[20](g(2*n))) od;
```

returns

$$1,\,1/4\sqrt{2},\,3-2\sqrt{2},\,1/4\sqrt{-14+10\sqrt{2}},\,9-4\sqrt{5},$$

for the first five even values of g_N^{-12}, but fails on the next three

0.034675177060507381314, 0.022419012334044683484,
0.014940167059400883091.

This can be remedied in many ways. For example,

```
 _EnvExplicit:=true:
   (PolynomialTools[MinimalPolynomial](g(14)^(1/3),4));
   solve(%)[2]; evalf(%/g(14)^(1/3));
```

yields $1-2X-5X^2-2X^3+X^4$ as the polynomial potentially satisfied by g_{14}^{-4}, and then extracts the correct radical

$$1/2+\sqrt{2}-1/2\sqrt{5+4\sqrt{2}},$$

which is confirmed to 15 places. One may check that $(g_{14}^6+g_{14}^{-6})/2=\sqrt{2}+1$ is an even simpler invariant. Similarly,

```
_EnvExplicit:=true:(PolynomialTools[MinimalPolynomial]
  (G(25)^(1/12),4));
```

illustrates that G_{25} solves $x^2-x-1=0$ and so is the golden mean, and it also shows that the appropriate power of G_N, g_N varies with N. When one is armed with these tools, a fine challenge is to obtain all values of G_N, g_N, or k_N up to, say, $N=50$.

We may now record two families of series of which Ramanujan discovered many cases:

Theorem 2.2 (Ramanujan-Type Series). [52, p. 182]
(a) For $N > 1$

$$\frac{1}{\pi} = \sum_{n=0}^{\infty} r_n^3 \left\{(\alpha_N - \sqrt{N} k_N^2) + n\sqrt{N}(k'^2_N - k_N^2)\right\} \left(G_N^{-12}\right)^{2n}. \tag{2.35}$$

(b) For $N \geq 1$

$$\frac{1}{\pi} = \sum_{n=0}^{\infty} (-1)^n r_n^3 \left\{\alpha_N k'^{-2}_N + n\sqrt{N}\frac{1+k_N^2}{1-k_N^2}\right\} \left(g_N^{-12}\right)^{2n}. \tag{2.36}$$

Example 2.3 (Identifying Our Series). We shall now try to determine which cases of Theorem 2.2 we have recovered.

Crude code to determine the coefficients is

```
A:=proc() local N;
   N:=args[1]; if nargs>1 then Digits:=args[2] fi;
   identify(evalf(G(N))),
   identify(evalf(a0(N)))+'n'*identify(evalf(a1(N))) end:

B:=proc() local N;
   N:=args[1]; if nargs>1 then Digits:=args[2] fi;
   identify(evalf(g(N))),
   identify(evalf(b0(N)))+'n'*identify(evalf(b1(N))) end:
```

for the nonalternating and alternating cases, respectively. For example, $B(1)$ returns $\sqrt{2}, 3n+1/4$ which means that

$$\frac{2}{\pi} = \sum_{n=0}^{\infty} (-1)^n r(n)^3 (1+4n).$$

We leave it to the reader to see that we had recovered the cases $N = 3, 5, 7, 15, 25$ and $N = 4, 6, 10, 18$ of Theorem 2.2(b). ◇

3 Algorithms for Experimental Mathematics II

Kronecker said, "In mathematics, I recognize true scientific value only in concrete mathematical truths, or to put it more pointedly, only in mathematical formulas." ... I would rather say "computations" than "formulas", but my view is essentially the same.

—Harold Edwards [124, p. 1]

3.1 True Scientific Value

One fascinating nonnumerical algorithm is the Wilf-Zeilberger (WZ) algorithm, which employs "creative telescoping" to show that a sum (with either finitely or infinitely many terms) is zero. We will not provide here any details of this remarkable procedure, which is now available for public usage. Interested readers are referred to the very readable book by Petkovsek, Wilf, and Zeilberger [229]. For most purposes, packages available in *Maple* and *Mathematica* suffice. Some other software implementing these schemes [281] is available from http://www.cis.upenn.edu/~wilf/progs.html.

As a simple example of the usage of this scheme, we first present a WZ proof of $(1+1)^n = 2^n$. This proof is from Doron Zeilberger's original *Maple* program, which in turn is inspired by the proof in [288].

Let $F(n,k) = \binom{n}{k}2^{-n}$. We wish to show that $L(n) = \sum_k F(n,k) = 1$ for every n. To this end, we construct, using the WZ algorithm, the function

$$G(n,k) \quad = \quad \frac{-1}{2^{(n+1)}}\binom{n}{k-1}\left(= \frac{-k}{2(n-k+1)}F(n,k)\right), \tag{3.1}$$

and observe that

$$F(n+1,k) - F(n,k) \quad = \quad G(n,k+1) - G(n,k). \tag{3.2}$$

By applying the obvious telescoping property of these functions, we can write

$$\begin{aligned} \sum_k F(n+1,k) - \sum_k F(n,k) &= \sum_k (G(n,k+1) - G(n,k)) \\ &= 0, \end{aligned}$$

which establishes that $L(n+1) - L(n) = 0$. The fact that $L(0) = 1$ follows from the fact that $F(0,k) = 1$ if $k = 0$ and 0 otherwise.

As a second example, we will briefly present here the proof of Guillera's identities, written here in a slightly different but equivalent form,

$$\sum_{n=0}^{\infty} \frac{\binom{4n}{2n}\binom{2n}{n}^4}{2^{16n}} \left(120n^2+34n+3\right) = \frac{32}{\pi^2},$$
$$\sum_{n=0}^{\infty} \frac{(-1)^n\binom{2n}{n}^5}{2^{20n}} \left(820n^2+180n+13\right) = \frac{128}{\pi^2},$$

which, as we mentioned in the previous chapter, can be discovered by a PSLQ-based search strategy.

Guillera [154] started by defining

$$G(n,k) = \frac{(-1)^k}{2^{16n}2^{4k}} \left(120n^2+84nk+34n+10k+3\right) \frac{\binom{2n}{n}^4\binom{2k}{k}^3\binom{4n-2k}{2n-k}}{\binom{2n}{k}\binom{n+k}{n}^2}. \tag{3.3}$$

He then used the software package EKHAD, which implements the WZ method, obtaining the companion formula

$$F(n,k) = \frac{(-1)^k 512}{2^{16n}2^{4k}} \frac{n^3}{4n-2k-1} \frac{\binom{2n}{n}^4\binom{2k}{k}^3\binom{4n-2k}{2n-k}}{\binom{2n}{k}\binom{n+k}{n}^2}. \tag{3.4}$$

Zeilberger's theorem [229, p. 25] says that when we define

$$H(n,k) = F(n+1,n+k)+G(n,n+k),$$

then it follows that

$$\sum_{n=0}^{\infty} G(n,0) = \sum_{n=0}^{\infty} H(n,0),$$

which when written out is

$$\begin{aligned}\sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4\binom{4n}{2n}}{2^{16n}} \left(120n^2+34n+3\right) &= \sum_{n=0}^{\infty} \frac{(-1)^n}{2^{20n+7}} \frac{(n+1)^3}{2n+3} \frac{\binom{2n+2}{n+1}^4\binom{2n}{n}^3\binom{2n+4}{n+2}}{\binom{2n+2}{n}\binom{2n+1}{n+1}^2} \\ &\quad + \sum_{n=0}^{\infty} \frac{(-1)^n}{2^{20n}} \left(204n^2+44n+3\right) \binom{2n}{n}^5 \\ &= \frac{1}{4}\sum_{n=0}^{\infty} \frac{(-1)^n\binom{2n}{n}^5}{2^{20n}} \left(820n^2+180n+13\right)\end{aligned}$$

after considerable algebra.

Guillera then observes that since $\sum_{n\geq 0} G(n,k) = \sum_{n\geq 0} G(n,k+1)$, then by Carlson's theorem [28] it follows that $\sum_{n\geq 0} G(n,k) = A$ for some A, independent of k, even if k is not an integer. We then note that $0 < G(n,t) \leq 8^{-n}$, so one can interchange limit and sum to conclude that

$$\lim_{t\to 1/2} \sum_{n=1}^{\infty} \mathrm{Re}\,[G(n,t)] \quad = \quad 0.$$

Thus,

$$A \quad = \quad \lim_{t\to 1/2} \mathrm{Re}\,[G(0,t)] \; = \; \frac{32}{\pi^2},$$

and we have

$$\sum_{n=0}^{\infty} G(n,k) \quad = \quad \sum_{n=0}^{\infty} H(n,k) \; = \; \frac{32}{\pi^2}.$$

Guillera's two results follow immediately.

Obviously, this proof does not provide much insight, since the difficult part of the result is buried in the construction of (3.3). In other words, the WZ method provides "proofs," but these proofs tend to be relatively unenlightening. Nonetheless, the very general nature of this scheme is of interest. It possibly presages a future in which a wide class of such identities can be proved automatically in a computer algebra system. Details and additional applications of this algorithm are given in [229].

3.2 Prime Number Computations

It is well known that there is a connection between prime numbers and the Riemann zeta function [50]. Prime numbers crop up in numerous other arenas of mathematical research, and often even in commercial applications, with the rise of RSA-based encryption methods on the Internet. Inasmuch as this research topic is certain to be of great interest for the foreseeable future, we mention here some of the techniques for counting, generating, and testing prime numbers.

The prime-counting function

$$\pi(x) \quad = \quad \#\{\text{primes} \leq x\}$$

is of central interest in this research. Table 3.1 gives $\pi(x)$ for power-of-ten arguments up to 10^{22}. This data was obtained from Eric Weisstein's "World of Mathematics" website [278].

It is clear from even a cursory glance at Table 3.1 that the researchers who have produced these counts are not literally testing every integer up to 10^{22} for primality—that would require much more computation than the combined power of all computers worldwide, even using the best-known methods to test individual primes. Indeed, some very sophisticated techniques have been employed, which unfortunately are too technical to be presented in detail here. We refer interested readers to the discussion of this topic in the book *Prime Numbers: A Computational Perspective* by Richard Crandall and Carl Pomerance [108, pp. 140–150]. Readers who wish to informally explore the behavior of $\pi(x)$ may use a sieving algorithm, which is a variant of a scheme originally presented by Eratosthenes of Cyrene about 200 BCE [108, p. 114].

If one does not require certainty, but only high probability, that a number is prime, some very efficient probabilistic primality tests have been discovered in the past few decades. In fact, these schemes are now routinely used to generate

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

Table 3.1. The prime-counting function $\pi(x)$ and Gauss' approximation.

primes for RSA encryption in Internet commerce. When you type in your Visa or Mastercard number in a secure website to purchase a book or computer accessory, somewhere in the process it is quite likely that two large prime numbers have been generated, which were certified as prime using one of these schemes.

The most widely used probabilistic primality test is the following, which was originally suggested by Artjuhov in 1966, although it was not appreciated until it was rediscovered and popularized by Selfridge in the 1970s [108].

Algorithm 3.1 (Strong Probable Prime Test). Given an integer $n = 1 + 2^s t$, for integers s and t (and t odd), select an integer a by means of a pseudorandom number generator in the range $1 < a < n - 1$.

1. Compute $b := a^t \bmod n$ using the binary algorithm for exponentiation (see Section 2.4.1 above; for an explicit formulation see Algorithm 3.2 in Chapter 3 of [50]). If $b = 1$ or $b = n - 1$, then exit (n is a strong probable prime base a).

2. For $j = 1$ to $s - 1$ do: Compute $b := b^2 \bmod n$; if $(b = n - 1)$, then exit (n is a strong probable prime base a).

3. Exit: n is composite.

This test can be repeated several times with different pseudorandomly chosen a. In 1980 Monier and Rabin independently showed that an integer n that passes the test as a strong probable prime is prime with probability at least $3/4$, so that m tests increase this probability to $1 - 1/4^m$ [214, 243]. In fact, for large test integers n, the probability is even closer to unity. Damgard, Landrock, and Pomerance showed in 1993 that if n has k bits, then this probability is greater than $1 - k^2 4^{2-\sqrt{k}}$, and for certain k is even higher [109]. For instance, if n has 500 bits, then the probability after m tests is greater than $1 - 1/4^{28m}$. Thus, a 500-bit integer that passes this test even once is prime with prohibitively safe odds—the chance of a false declaration of primality is less than one part in Avogadro's number (6×10^{23}). If it passes the test for four pseudorandomly chosen integers a, then the chance of false declaration of primality is less than one part in a googol (10^{100}). Such probabilities are many orders of magnitude more remote than the chance that an undetected hardware or software error has occurred in the computation.

How many primes are generated by these algorithms each day? Let us assume for point of discussion that this is roughly the same as the number of online secure transactions performed each day (since with each such transaction at least one and possibly two large primes are generated, depending on whether RSA or Diffe-Hellman PKC is being used). Then, based on the information given in [273], we estimate that at least five million secure online transactions per day are performed at the present time (July 2006), so that more than this number of large primes are generated each day. But note also that, again according to the information cited above, online transactions are increasing in number and in dollar volume at roughly a 30% per year rate!

A number of more advanced probabilistic primality testing algorithms are now known. The current state-of-the-art is that such tests can determine the primality of integers with hundreds to thousands of digits. Additional details of these schemes are available in [108].

For these reasons, probabilistic primality tests are considered entirely satisfactory for practical use, even for applications such as large interbank financial transactions, which have extremely high security requirements. Nonetheless, mathematicians have long sought tests that remove this last iota of uncertainty, yielding a mathematically rigorous certificate of primality. Indeed, the question of whether there exists a "polynomial time" primality test has long stood as an important unsolved question in pure mathematics.

Thus, it was with considerable elation that such an algorithm was recently discovered, by Manindra Agrawal, Neeraj Kayal, and Nitin Saxena (initials AKS) of the Indian Institute of Technology in Kanpur, India [2]. Their discovery sparked worldwide interest, including a prominent report in the *New York Times* [248]. Since the initial report in August 2002, several improvements have been made. Readers are referred to a variant of the original algorithm due to Lenstra [197], as implemented by Richard Crandall and Jason Papadopoulos [107, 51, p. 303].

3.3 Roots of Polynomials

In Chapter 2, we mentioned that Newton iterations can be used to compute high-precision square roots and divisions. This Newton iteration scheme is, in fact, quite general and can be used to solve many kinds of equations, both algebraic and transcendental. One particularly useful application, frequently encountered by experimental mathematicians, is to find roots of polynomials. This is done by using a careful implementation of the well-known version of Newton's iteration

$$x_{k+1} = x_k - \frac{p(x)}{p'(x)}, \tag{3.5}$$

where $p'(x)$ denotes the derivative of $p(x)$. As before, this scheme is most efficient if it employs a level of numeric precision that starts with ordinary double precision (16-digit) or double-double precision (32-digit) arithmetic until convergence is achieved at this level, then approximately doubles with each iteration until the final level of precision is attained. One additional iteration at the penultimate or final precision level may be needed to insure full accuracy.

Note that Newton's iteration can be performed, as written in (3.5), with either real or complex arithmetic, so that complex roots of polynomials (with real or complex coefficients) can be found almost as easily as real roots. Evaluation of the polynomials $p(x)$ and $p'(x)$ is most efficiently performed using Horner's rule: For example, the polynomial $p(x) = p_0 + p_1x + p_2x^2 + p_3x^3 + p_4x^4 + p_5x^5$ is evaluated as $p(x) = p_0 + x(p_1 + x(p_2 + x(p_3 + x(p_4 + xp_5))))$.

There are two issues that arise here that do not arise with the Newton iteration schemes for division and square root. The first is the selection of the starting value—if it is not close to the desired root, then successive iterations may jump far away. If you have no idea where the roots are (or how accurate the starting value must be), then a typical strategy is to try numerous starting values, covering a wide range of likely values, and then make an inventory of the approximate roots that are found. If you are searching for complex roots, note that it is often necessary to use a two-dimensional array of starting values. These exploratory iterations can be done quite rapidly, since typically only a modest numeric precision is required—in almost all cases, just ordinary double precision (16 digits) or double-double precision (32 digits) arithmetic will do. Once the roots have been located in this fashion, then the full-fledged Newton scheme can be used to produce their precise high-precision values.

The second issue is how to handle repeated roots. The difficulty here is that, in such cases, convergence to the root is very slow, and instabilities may throw the search far from the root. In these instances, note that we can write $p(x) = q^2(x)r(x)$, where r has no repeated roots (if all roots are repeated an even number of times, then $r(x) = 1$). Now note that $p'(x) = 2q(x)r(x) + q^2(x)r'(x) = q(x)[2r(x) + q(x)r'(x)]$. This means that if $p(x)$ has repeated roots, then these roots are also roots of $p'(x)$, and, conversely, if $p(x)$ and $p'(x)$ have a common factor, then the roots of this common factor are repeated roots of $p(x)$. This greatest common divisor polynomial $q(x)$ can be found by performing the Euclidean algorithm (in the ring of polynomials) on $p(x)$ and $p'(x)$. The Newton iteration scheme can then be applied to find the roots of both $q(x)$ and $r(x)$. It is possible, of course, that $q(x)$ also has repeated roots, but recursive application of this scheme quickly yields all individual roots.

In the previous paragraph, we mentioned the possible need to perform the Euclidean algorithm on two polynomials, which involves polynomial multiplication and division. For modest-degree polynomials, a simple implementation of the schemes learned in high-school algebra suffices—just represent the polynomials as strings of high-precision numbers. For high-degree polynomials, polynomial multiplication can be accelerated by utilizing fast Fourier transforms and a convolution scheme that is almost identical to the scheme, mentioned in Chapter 2, to perform high-precision multiplication. High-degree polynomial division can be accelerated by a Newton iteration scheme, similar to that mentioned above for high-precision division. See [108] for additional details on high-speed polynomial arithmetic. One other approach to computing roots of polynomials is to cast the problem as an eigenvalue problem and apply QR iterations [123].

We noted above that if the starting value is not quite close to the desired root, then successive Newton iterations may jump far from the root, and eventually converge to a different root than the one desired. In general, suppose that we are given a degree-n polynomial $p(x)$ with m distinct complex roots r_k (some may be repeated roots). Define the function $Q_p(z)$ as the limit achieved by successive Newton iterations that start at the complex number z; if no limit is achieved, then set $Q_p(z) = \infty$. Then the m sets $\{z : Q_p(z) = r_k\}$ for $k = 1,2\cdots,m$ constitute a partition of the complex plane, except for a filamentary set of measure zero that separates the m sets. In fact, each of these m sets is itself an infinite collection of disconnected components.

The collection of these Newton-Julia sets and their boundaries form pictures of striking beauty and are actually quite useful in gaining insight on both the root

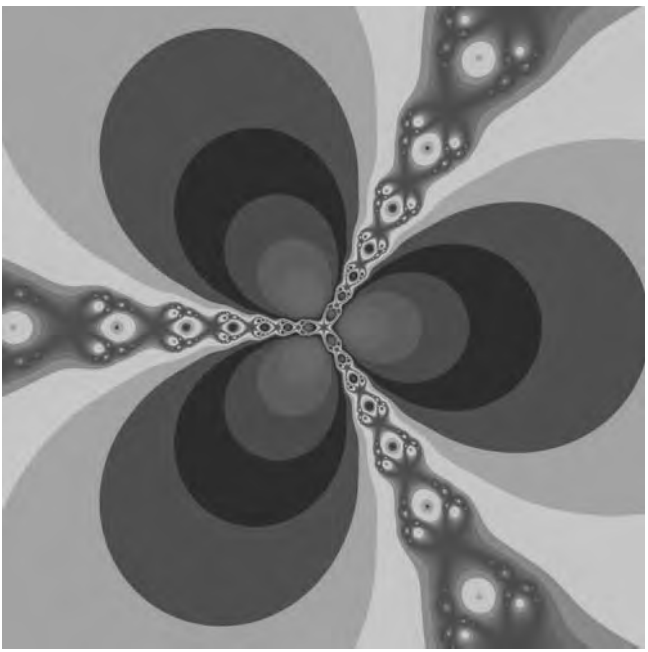


Figure 3.1. Newton-Julia set for $p(x) = x^3 - 1$.

structure of the original polynomial and the behavior of Newton iteration solutions. Some of the most interesting graphics of this type are color-coded plots of the function $N_p(z)$, which is the number of iterations required for convergence (to some accuracy ε) of Newton's iteration for $p(x)$, beginning at z (if the Newton iteration does not converge at z, then set $N_p(z) = \infty$). A plot for the cubic polynomial $p(x) = x^3 - 1$ is shown in Figure 3.1.

3.4 Numerical Quadrature

Experimental mathematicians very frequently find it necessary to calculate definite integrals to high precision. Recall the example given in Chapter 2, wherein we were able to experimentally identify certain definite integrals as analytic expressions, based only on their high-precision numerical value. As a second example, two of the present authors (Bailey and Borwein) empirically determined that

$$\begin{aligned}\frac{2}{\sqrt{3}}\int_0^1 \frac{\log^6(x)\arctan[x\sqrt{3}/(x-2)]}{x+1}\,dx \\ = \frac{1}{81648}\Big[-229635L_{-3}(8) + 29852550L_{-3}(7)\log 3 - 1632960L_{-3}(6)\pi^2 \\ + 27760320L_{-3}(5)\zeta(3) - 275184L_{-3}(4)\pi^4 + 36288000L_{-3}(3)\zeta(5) \\ - 30008L_{-3}(2)\pi^6 - 57030120L_{-3}(1)\zeta(7)\Big],\end{aligned}$$

where $L_{-3}(s) = \sum_{n=1}^{\infty}\left[1/(3n-2)^s - 1/(3n-1)^s\right]$. General results have been conjectured but not yet rigorously established.

A third result is the following, which was found by one of the present authors (Borwein) and British physicist David Broadhurst [61]:

$$\begin{aligned}\frac{24}{7\sqrt{7}}\int_{\pi/3}^{\pi/2} \log\left|\frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}}\right| dt \stackrel{?}{=} L_{-7}(2) \\ = \sum_{n=0}^{\infty}\Big[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} \\ + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2}\Big]. \qquad (3.6)\end{aligned}$$

This integral arose out of some studies in quantum field theory, in analysis of the volume of ideal tetrahedra in hyperbolic space, and it was mentioned already in Chapter 1. It is the simplest of 998 empirically determined cases where the volume of a hyperbolic knot complement is expressible in terms of an L-series and an apparently unexpected integral or sum [61]. The question mark is used here because, although this identity has been numerically verified to 20,000-digit precision using the tanh-sinh quadrature scheme that we will describe below, as of this date no proof is yet known.

PSLQ computations were also able to recover relations among integrals of this type. Let I_n be the definite integral of (3.6), except with limits $n\pi/24$ and $(n+1)\pi/24$. Then the relations

$$\begin{aligned} -2I_2 - 2I_3 - 2I_4 - 2I_5 + I_8 + I_9 - I_{10} - I_{11} &\stackrel{?}{=} 0, \\ I_2 + 3I_3 + 3I_4 + 3I_5 + 2I_6 + 2I_7 - 3I_8 - I_9 &\stackrel{?}{=} 0 \end{aligned} \tag{3.7}$$

have been numerically discovered, although as before no hint of a proof is known.

As a fourth example, recently two of the present authors (Bailey and Borwein) together with Richard Crandall were studying the following integrals, which are related to Ising theory of mathematical physics:

$$C_n = \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}.$$

At present, there is no known practical scheme to find high-precision values of general iterated integrals. However, Crandall showed that in this case

$$C_n = \frac{2^n}{n!}\int_0^\infty t K_0^n(t)\, dt,$$

where $K_0(t)$ denotes the modified Bessel function, thus reducing the problem to one-dimensional integrals that are amenable to high-precision quadrature.

We then computed high-precision values (up to 1000 digits) for selected values of n, ranging from 3 up to 1024 (corresponding to a 1024-fold iterated integral). With these numerical values in hand, we were able to find and then prove the following intriguing results [18]:

$$\begin{aligned} C_3 &= \mathrm{L}_{-3}(2) = \sum_{n\geq 0}\left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2}\right), \\ C_4 &= 14\zeta(3), \\ \lim_{n\to\infty} C_n &= 2e^{-2\gamma}, \end{aligned}$$

where γ is the Euler-Mascheroni constant

$$\gamma := \lim_{n\to\infty} 1 + \frac{1}{2} + \frac{1}{3} + \cdots \frac{1}{n} - \log n.$$

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 a state-of-the-art, highly efficient technique for numerical quadrature. Some additional schemes and refinements, not mentioned here, are described in [26]. You can try programming these schemes yourself, or you can refer to the C++ and Fortran-90 programs available at [15].

3.4.1 Tanh-Sinh Quadrature

The scheme we will discuss here is known as *tanh-sinh quadrature*. While it 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. Also, the cost of computing abscissas and weights in tanh-sinh quadrature only scales as $p^2 \log p$ in tanh-sinh quadrature, where p is the number of correct digits in the result (for many problems), whereas the corresponding cost for Gaussian quadrature scales as $p^3 \log p$. For this reason, Gaussian quadrature is not practical beyond about 1,000 digits.

The tanh-sinh quadrature scheme is based on the Euler-Maclaurin summation formula, which can be stated as follows [9, p. 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

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

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

$$E(h,m) = \frac{h^{2m+2}(b-a) B_{2m+2} f^{(2m+2)}(\xi)}{(2m+2)!}, \tag{3.8}$$

for some $\xi \in (a,b)$. Remember that the Bernoulli numbers, given by the series

$$\frac{x}{e^x - 1} = 1 - \frac{1}{2}x + \sum_{n=1}^{\infty} B_{2n} \frac{x^{2n}}{(2n)!}, \tag{3.9}$$

are rational numbers with alternating signs.

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 $E(h,m)$. 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 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 $h > 0$,

$$\int_{-1}^{1} f(x)\,dx \quad = \quad \int_{-\infty}^{\infty} f(g(t))g'(t)\,dt \approx h\sum_{-\infty}^{\infty} w_j f(x_j), \tag{3.10}$$

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 tanh-sinh scheme employs the transformation $x = \tanh(\pi/2 \cdot \sinh t)$, where $\sinh t = (e^t - e^{-t})/2$, $\cosh t = (e^t + e^{-t})/2$, and $\tanh t = \sinh t/\cosh t$ (alternately, one can omit the $\pi/2$ in this definition). This transformation converts an integral on $(-1,1)$ to an integral on the entire real line, which can then be approximated by means of a simple step-function summation. In this case, by differentiating the transformation, we obtain the abscissas x_k and the weights w_k as

$$\begin{aligned} x_j &= \tanh[\pi/2 \cdot \sinh(jh)], \\ w_j &= \frac{\pi/2 \cdot \cosh(jh)}{\cosh^2[\pi/2 \cdot \sinh(jh)]}. \end{aligned} \tag{3.11}$$

Note that these functions involved here are compound exponential, so, for example, the weights w_j converge very rapidly to zero. As a result, the tanh-sinh quadrature scheme is often very effective in dealing with singularities or infinite derivatives at endpoints.

Algorithm 3.2 (Tanh-Sinh Quadrature).
Initialize: Set $h := 2^{-m}$.
For $k := 0$ to $20 \cdot 2^m$ do:
Set $t := kh$, $x_k := \tanh(\pi/2 \cdot \sinh t)$, and $w_k := \pi/2 \cdot \cosh t / \cosh^2(\pi/2 \cdot \sinh t)$;
If $|x_k - 1| < \varepsilon$ 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 $h := 1$.
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 $(\bmod(i, 2^{m-k+1}) \neq 0$ 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; enddo.
Result $= hS$.

There are several similar quadrature schemes that can be defined, also based on the Euler-Maclaurin summation formula. For example, using $g(t) = \mathrm{erf}(t)$ gives rise to *error function* or *erf* quadrature; using $g(t) = \sinh(\sinh t)$ gives rise to *sinh-sinh* quadrature, which can be used for functions defined on the entire real line. Additional refinements are described in [26]. An implementation of this scheme on a highly parallel computer system is described in [14].

3.4.2 Practical Considerations for Quadrature

So far we have assumed a function of one variable defined and continuous on the interval $(-1,1)$. Integrals on other finite intervals (a,b) can be found by applying a linear change of variable

$$\int_a^b f(t)\,dt = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b+a}{2} + \frac{b-a}{2}x\right) dx. \tag{3.12}$$

Note also that integrable functions on an infinite interval can, in a similar manner, be reduced to an integral on a finite interval: for example,

$$\int_0^\infty f(t)\,dt \quad = \quad \int_0^1 [f(x) + f(1/x)/x^2]\,dx. \tag{3.13}$$

Integrals of functions with singularities (such as corners or step discontinuities) within the integration interval (i.e., not at the endpoints) should be broken into separate integrals.

The above algorithm statement suggests increasing the level of the quadrature (the value of k) until two successive levels give the same value of S, to within some tolerance ε. While this is certainly a reliable termination test, it is often possible to stop the calculation earlier, with significant savings in runtime, by means of making reasonable projections of the current error level. In this regard, the authors have found the following scheme to be fairly reliable: Let S_1, S_2, and S_3 be the value of S at the current level, the previous level, and two levels back, respectively. Then set $D_1 := \log_{10}|S_1 - S_2|$, $D_2 := \log_{10}|S_1 - S_3|$, and $D_3 := \log_{10}\varepsilon - 1$. Now we can estimate the error E at level $k > 2$ as 10^{D_4}, where $D_4 = \min(0, \max(D_1^2/D_2, 2D_1, D_3))$. These estimation calculations may be performed using ordinary double precision arithmetic.

In the case of tanh-sinh quadrature (or other schemes based on the Euler-Maclaurin summation formula as above), the following formula provides a more accurate estimate of the error term. Let $F(t)$ be the desired integrand function, and then define $f(t) = F(g(t))g'(t)$, where $g(t) = \tanh(\sinh t)$ (or one could use any of the other g functions mentioned above). Then consider

$$E_2(h,m) \quad = \quad h(-1)^{m-1}\left(\frac{h}{2\pi}\right)^{2m} \sum_{j=a/h}^{b/h} D^{2m} f(jh). \tag{3.14}$$

In many cases, this estimate of the error term is exceedingly accurate once h is moderately small, for any integer $m \geq 1$. In most cases, it is sufficient to use $E_2(h,1)$, although higher-order estimates can be used with the bound

$$|E(h,m) - E_2(h,m)| \\ \leq 2\left[\zeta(2m) + (-1)^m \zeta(2m+2)\right]\left(\frac{h}{2\pi}\right)^{2m} h\sqrt{\int_a^b |D^{2m} f(t)|^2\,dt},$$

to yield rigorous certificates of quadrature results. See [12] for details.

Some refinements to these schemes, and to the error estimation procedure above, are described in [26, 12]. The tanh-sinh scheme has been implemented in C++ and Fortran-90 programs, available at [15].

3.4.3 Higher-Dimensional Quadrature

The tanh-sinh quadrature scheme can be easily generalized to perform two-dimensional (2-D) and three-dimensional (3-D) quadrature. Runtimes are typically many times higher than with one-dimensional (1-D) integrals. However, if one is content with, say, 32-digit or 64-digit results (by using double-double or quad-double arithmetic, respectively), then many two-variable functions can be integrated in reasonable runtime (say, a few minutes). One advantage that these schemes have is that they are very well suited to parallel processing. Thus, even several-hundred digit values can be obtained for 2-D and 3-D integrals if one can utilize a highly parallel computer, such as a Beowulf cluster. One can even envision harnessing many computers on a geographically distributed grid for such a task, although the authors are not aware of any such attempts yet.

3.5 Infinite Series Summation

We have already seen numerous examples in previous chapters of mathematical constants defined by infinite series. In experimental mathematics, it is usually necessary to evaluate such constants to several hundred digit accuracy. The commercial software packages *Maple* and *Mathematica* include quite good facilities for the numerical evaluation of series. However, as with numerical quadrature, these packages do have limitations, and in some cases better results can be obtained using custom-written computer code. In addition, even if one relies exclusively on these commercial packages, it is useful to have some idea of the sorts of operations that are being performed by such software.

Happily, in many cases of interest to the experimental mathematician, infinite series converge sufficiently rapidly that they can be numerically evaluated to high precision by simply evaluating the series directly as written, stopping the summation when the individual terms are smaller than the epsilon of the multiprecision arithmetic system being used. All of the BBP-type formulas, for instance, are of this category. But other types of infinite series formulas present considerable difficulties for high-precision evaluation. Two simple examples are Gregory's series for $\pi/4$ and a similar series for Catalan's constant:

$$
\begin{aligned}
\pi &= 1 - 1/3 + 1/5 - 1/7 + \cdots, \\
G &= 1 - 1/3^2 + 1/5^2 - 1/7^2 + \cdots .
\end{aligned}
$$

We describe here one technique that is useful in many such circumstances. In fact, we have already been introduced to it in an earlier section of this chapter: It is the Euler-Maclaurin summation formula. The Euler-Maclaurin formula can be written in somewhat different form than before, as follows [9, p. 282]. Let $m \geq 0$ be an integer, and assume that the function $f(x)$ is at least $(2m+2)$-times continuously differentiable on $[a,\infty)$ and that $f(x)$ and all of its derivatives approach zero for large x. Then

$$\sum_{j=a}^{\infty} f(j) \quad = \quad \int_a^{\infty} f(x)\,dx + \frac{1}{2} f(a) - \sum_{i=1}^{m} \frac{B_{2i}}{(2i)!} f^{(2i-1)}(a) + E, \tag{3.15}$$

where, as before, B_{2i} denotes the Bernoulli numbers and

$$E \quad = \quad \frac{B_{2m+2}\, f^{(2m+2)}(\xi)}{(2m+2)!}, \tag{3.16}$$

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

This formula is not effective as written. The strategy is instead to evaluate a series manually for several hundred or several thousand terms, then to use the Euler-Maclaurin formula to evaluate the tail. Before giving an example, we need to describe how to calculate the Bernoulli numbers B_{2k}, which are required here. The simplest way to compute them is to recall that [1, p. 807]

$$\zeta(2k) \quad = \quad (-1)^{k+1} \frac{(2\pi)^{2k} B_{2k}}{2(2k)!}, \tag{3.17}$$

which can be rewritten as

$$\frac{B_{2k}}{(2k)!} \quad = \quad \frac{2(-1)^{k+1}\zeta(2k)}{(2\pi)^{2k}}. \tag{3.18}$$

The Riemann zeta function at real arguments s can, in turn, be computed using the formula [73]

$$\zeta(s) \quad = \quad \frac{-1}{2^n(1-2^{1-s})} \sum_{j=0}^{2n-1} \frac{e_j}{(j+1)^s} + E_n(s), \tag{3.19}$$

where

$$e_j \quad = \quad (-1)^j \left(\sum_{k=0}^{j-n} \frac{n!}{k!(n-k)!} - 2^n \right) \tag{3.20}$$

(the summation is zero when its index range is null) and

$$|E_n(s)| < 1/(8^n |1-2^{1-s}|).$$

This scheme is encapsulated in the following algorithm.

Algorithm 3.3 (Zeta Function Evaluation).
Initialize: Set $n = P/3$, where P is the precision level in bits, and set $t_1 := -2^n$, $t_2 := 0$, $S := 0$, and $I = 1$.

For $j := 0$ to $2n-1$ do:
If $j < n$ then $t_2 := 0$
elseif $j = n$ then $t_2 := 1$ else $t_2 := t_2 \cdot (2n - j + 1)/(j - n)$
endif.

Set $t_1 := t_1 + t_2$, $S := S + I \cdot t_1/(j+1)^s$, and $I := -I$; enddo.
Return $\zeta(s) := -S/[2^n \cdot (1 - 2^{1-s})]$.

A more advanced method to compute the zeta function in the particular case of interest here, where we need the zeta function evaluated at all even integer arguments up to some level m, is described in [17].

We illustrate the above by calculating Catalan's constant using the Euler-Maclaurin formula. We can write

$$\begin{aligned}
G &= (1 - 1/3^2) + (1/5^2 - 1/7^2) + (1/9^2 - 1/11^2) + \cdots \\
&= 8 \sum_{k=0}^{\infty} \frac{2k+1}{(4k+1)^2(4k+3)^2} \\
&= 8 \sum_{k=0}^{n} \frac{2k+1}{(4k+1)^2(4k+3)^2} + 8 \sum_{k=n+1}^{\infty} \frac{2k+1}{(4k+1)^2(4k+3)^2} \\
&= 8 \sum_{k=0}^{n} \frac{2k+1}{(4k+1)^2(4k+3)^2} + 8 \int_{n+1}^{\infty} f(x)\,dx + 4f(n+1) \\
&\quad -8 \sum_{i=1}^{m} \frac{B_{2i}}{(2i)!} f^{(2i-1)}(n+1) + 8E,
\end{aligned}$$

where $f(x) = (2x+1)/[(4x+1)^2(4x+3)^2]$ and $|E| < 3/(2\pi)^{2m+2}$. Using $m = 20$ and $n = 1000$ in this formula, we obtain a value of G correct to 114 decimal digits. We presented the above scheme for Catalan's constant because it is illustrative of the Euler-Maclaurin method. However, serious computation of Catalan's constant can be done more efficiently using the recently discovered BBP-type formula (given in Table 3.5 of [50]), Ramanujan's formula (given in Item 7 of Chapter 6 in [50]), or Bradley's formula (also given in Item 7 of Chapter 6 in [50]).

One less-than-ideal feature of the Euler-Maclaurin approach is that high-order derivatives are required. In many cases of interest, successive derivatives satisfy a fairly simple recursion and can thus be easily computed with an ordinary hand-written computer program. In other cases, these derivatives are sufficiently complicated that such calculations are more conveniently performed in a symbolic computing environment such as *Mathematica* or *Maple*. In a few applications of this approach, a combination of symbolic computation and custom-written numerical computation is required to produce results in reasonable runtime [20].

3.6 Apéry-Like Summations

Here we present a detailed case study in identifying sums of a certain class of infinite series, by means of a multistep approach that is broadly illustrative of the experimental methodology in mathematics. The origins of this work lay in the existence of infinite series formulas involving central binomial coefficients in the denominators for the constants $\zeta(2)$, $\zeta(3)$, and $\zeta(4)$. These formulas, as well as the role of the formula for $\zeta(3)$ in Apéry's proof of its irrationality, have prompted considerable effort during the past few decades to extend these results to larger integer arguments. The formulas in question are

$$\zeta(2) = 3\sum_{k=1}^{\infty}\frac{1}{k^2\binom{2k}{k}}, \tag{3.21}$$

$$\zeta(3) = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}, \tag{3.22}$$

$$\zeta(4) = \frac{36}{17}\sum_{k=1}^{\infty}\frac{1}{k^4\binom{2k}{k}}. \tag{3.23}$$

Identity (3.21) has been known since the nineteenth century, while (3.22) was variously discovered in the last century and (3.23) was noted by Comtet [105, 62, 271].

These results led many to conjecture that the constant $\mathcal{Q}_5$ defined by the ratio

$$\mathcal{Q}_5 := \zeta(5)\Big/\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}}$$

is rational, or at least algebraic. However, 10,000-digit PSLQ computations have established that if $\mathcal{Q}_5$ is a zero of a polynomial of degree at most 25 with integer coefficients, then the Euclidean norm of the vector of coefficients exceeds 1.24×10^{383}. Similar computations for $\zeta(5)$ have yielded a bound of 1.98×10^{380}. These computations lend credence to the belief that $\mathcal{Q}_5$ and $\zeta(5)$ are transcendental.

Given the negative result from PSLQ computations for $\mathcal{Q}_5$, the authors of [56] systematically investigated the possibility of a multiterm identity of this general form for $\zeta(2n+1)$. The following were recovered early in experimental searches using computer-based integer relation tools [56, 55]:

$$\zeta(5) = 2\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}} - \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2}, \tag{3.24}$$

$$\zeta(7) = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}} + \frac{25}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}, \tag{3.25}$$

$$\begin{aligned}\zeta(9) = {} & \frac{9}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^9\binom{2k}{k}} - \frac{5}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2} \\ & +5\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4} + \frac{45}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^6} \\ & -\frac{25}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}\sum_{j=1}^{k-1}\frac{1}{j^2},\end{aligned} \tag{3.26}$$

$$\begin{aligned}\zeta(11) = {} & \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^{11}\binom{2k}{k}} + \frac{25}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4} \\ & -\frac{75}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^8} \\ & +\frac{125}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}\sum_{i=1}^{k-1}\frac{1}{i^4}.\end{aligned} \tag{3.27}$$

The general formula

$$\sum_{k=1}^{\infty}\frac{1}{k(k^2-x^2)} = \frac{1}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\frac{5k^2-x^2}{k^2-x^2}\prod_{m=1}^{k-1}\left(1-\frac{x^2}{m^2}\right) \tag{3.28}$$

was obtained by Koecher [183] following techniques of Knopp and Schur.

Using bootstrapping and an application of the `Pade` function (which in both *Mathematica* and *Maple* produces Padé approximations to a rational function satisfied by a truncated power series), the following remarkable and unanticipated result was produced [56]:

$$\sum_{k=1}^{\infty}\frac{1}{k^3(1-x^4/k^4)} = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}(1-x^4/k^4)}\prod_{m=1}^{k-1}\left(\frac{1+4x^4/m^4}{1-x^4/m^4}\right). \tag{3.29}$$

Following an analogous—but more deliberate—experimental-based procedure, as detailed below, we provide a similar general formula for $\zeta(2n+2)$ that is pleasingly parallel to (3.29). It is

Theorem 3.4. *Let x be a complex number not equal to a nonzero integer. Then*

$$\sum_{k=1}^{\infty} \frac{1}{k^2 - x^2} = 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k} (1 - x^2/k^2)} \prod_{m=1}^{k-1} \left(\frac{1 - 4x^2/m^2}{1 - x^2/m^2} \right). \tag{3.30}$$

Note that the left-hand side of (3.30) is equal to

$$\sum_{n=0}^{\infty} \zeta(2n+2)x^{2n} \quad = \quad \frac{1 - \pi x \cot(\pi x)}{2x^2}. \tag{3.31}$$

Thus, (3.30) generates an Apéry-like formulas for $\zeta(2n)$ for every positive integer n.

We describe this process of discovery in some detail here, as the general technique appears to be quite fruitful and may well yield results in other settings.

We first conjectured that $\zeta(2n+2)$ is a rational combination of terms of the form

$$\sigma(2r; [2a_1, \cdots, 2a_N]) \quad := \quad \sum_{k=1}^{\infty} \frac{1}{k^{2r} \binom{2k}{k}} \prod_{i=1}^{N} \sum_{n_i=1}^{k-1} \frac{1}{n_i^{2a_i}}, \tag{3.32}$$

where $r + \sum_{i=1}^{N} a_i = n+1$ and the a_i are listed in nonincreasing order (note that the right-hand-side value is independent of the order of the a_i). This dramatically reduces the size of the search space, while in addition the sums (3.32) are relatively easy to compute.

One can then write

$$\sum_{n=0}^{\infty} \zeta(2n+2)x^{2n} \quad \stackrel{?}{=} \quad \sum_{n=0}^{\infty} \sum_{r=1}^{n+1} \sum_{\pi \in \Pi(n+1-r)} \alpha(\pi)\, \sigma(2r; 2\pi)\, x^{2n}, \tag{3.33}$$

where $\Pi(m)$ denotes the set of all additive partitions of m if $m > 0$, $\Pi(0)$ is the singleton set whose sole element is the null partition $[\,]$, and the coefficients $\alpha(\pi)$ are complex numbers. In principle $\alpha(\pi)$ in (3.33) could depend not only on the partition π but also on n. However, since the first few coefficients appeared to be independent of n, we found it convenient to assume that the generating function could be expressed in the form given above.

For positive integer k and partition $\pi = (a_1, a_2, \ldots, a_N)$ of the positive integer m, let

$$\widehat{\sigma}_k(\pi) \quad := \quad \prod_{i=1}^{N} \sum_{n_i=1}^{k-1} \frac{1}{n_i^{2a_i}}.$$

Then

$$\sigma(2r; 2\pi) \quad = \quad \sum_{k=1}^{\infty} \frac{\widehat{\sigma}_k(\pi)}{k^{2r} \binom{2k}{k}},$$

and from (3.33) we deduce that

$$\begin{aligned}\sum_{n=0}^{\infty}\zeta(2n+2)x^{2n} &= \sum_{n=0}^{\infty}\sum_{r=1}^{n+1}\sum_{\pi\in\Pi(n+1-r)}\alpha(\pi)\sigma(2r;2\pi)x^{2n}\\ &= \sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}}\sum_{r=1}^{\infty}\frac{x^{2r-2}}{k^{2r}}\sum_{n=r-1}^{\infty}\sum_{\pi\in\Pi(n+1-r)}\alpha(\pi)\,\widehat{\sigma}_k(\pi)x^{2(n+1-r)}\\ &= \sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}(k^2-x^2)}\sum_{m=0}^{\infty}x^{2m}\sum_{\pi\in\Pi(m)}\alpha(\pi)\,\widehat{\sigma}_k(\pi)\\ &= \sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}(k^2-x^2)}P_k(x),\end{aligned}$$

where

$$P_k(x) := \sum_{m=0}^{\infty}x^{2m}\sum_{\pi\in\Pi(m)}\alpha(\pi)\,\widehat{\sigma}_k(\pi), \tag{3.34}$$

whose closed form is yet to be determined. Our strategy, as in the case of (3.29) [55], was to compute $P_k(x)$ explicitly for a few small values of k in a hope that these would suggest a closed form for general k.

Some examples we produced are shown below. At each step we bootstrapped by assuming that the first few coefficients of the current result are the coefficients of the previous result. Then we found the remaining coefficients (which are in each case unique) by means of PSLQ computations. Note below that in the sigma notation the first few coefficients of each expression are simply the previous step's terms, where the first argument of σ (corresponding to r) has been increased by two. These initial terms (with coefficients in bold) are then followed by terms with the other partitions as arguments, with all terms ordered lexicographically by partition (shorter partitions are listed before longer partitions, and, within a partition of a given length, larger entries are listed before smaller entries in the first position where they differ; the integers in brackets are nonincreasing):

$$\zeta(2) = 3\sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}k^2} = 3\sigma(2,[0]), \tag{3.35}$$

$$\zeta(4) = \mathbf{3}\sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}k^4} - 9\sum_{k=1}^{\infty}\frac{\sum_{j=1}^{k-1}j^{-2}}{\binom{2k}{k}k^2} = \mathbf{3}\sigma(4,[0]) - 9\sigma(2,[2]), \tag{3.36}$$

$$\begin{aligned}\zeta(6) = \mathbf{3}\sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}k^6} - \mathbf{9}\sum_{k=1}^{\infty}\frac{\sum_{j=1}^{k-1}j^{-2}}{\binom{2k}{k}k^4} - \frac{45}{2}\sum_{k=1}^{\infty}\frac{\sum_{j=1}^{k-1}j^{-4}}{\binom{2k}{k}k^2}\\ + \frac{27}{2}\sum_{k=1}^{\infty}\sum_{j=1}^{k-1}\frac{\sum_{i=1}^{k-1}i^{-2}}{j^2\binom{2k}{k}k^2}\end{aligned} \tag{3.37}$$

$$= \mathbf{3}\sigma(6,[]) - \mathbf{9}\sigma(4,[2]) - \frac{45}{2}\sigma(2,[4]) + \frac{27}{2}\sigma(2,[2,2]), \tag{3.38}$$

$$\begin{aligned}\zeta(8) &= \mathbf{3}\sigma(8,[]) - \mathbf{9}\sigma(6,[2]) - \frac{\mathbf{45}}{\mathbf{2}}\sigma(4,[4]) + \frac{\mathbf{27}}{\mathbf{2}}\sigma(4,[2,2]) \\ &\quad - 63\sigma(2,[6]) + \frac{135}{2}\sigma(2,[4,2]) - \frac{27}{2}\sigma(2,[2,2,2]),\end{aligned} \tag{3.39}$$

$$\begin{aligned}\zeta(10) &= \mathbf{3}\sigma(10,[]) - \mathbf{9}\sigma(8,[2]) - \frac{\mathbf{45}}{\mathbf{2}}\sigma(6,[4]) + \frac{\mathbf{27}}{\mathbf{2}}\sigma(6,[2,2]) \\ &\quad - \mathbf{63}\sigma(4,[6]) + \frac{\mathbf{135}}{\mathbf{2}}\sigma(4,[4,2]) - \frac{\mathbf{27}}{\mathbf{2}}\sigma(4,[2,2,2]) \\ &\quad - \frac{765}{4}\sigma(2,[8]) + 189\sigma(2,[6,2]) + \frac{675}{8}\sigma(2,[4,4]) \\ &\quad - \frac{405}{4}\sigma(2,[4,2,2]) + \frac{81}{8}\sigma(2,[2,2,2,2]).\end{aligned}$$

Partition	Alpha	Partition	Alpha	Partition	Alpha
[empty]	3/1	1	-9/1	2	-45/2
1,1	27/2	3	-63/1	2,1	135/2
1,1,1	-27/2	4	-765/4	3,1	189/1
2,2	675/8	2,1,1	-405/4	1,1,1,1	81/8
5	-3069/5	4,1	2295/4	3,2	945/2
3,1,1	-567/2	2,2,1	-2025/8	2,1,1,1	405/4
1,1,1,1,1	-243/40	6	-4095/2	5,1	9207/5
4,2	11475/8	4,1,1	-6885/8	3,3	1323/2
3,2,1	-2835/2	3,1,1,1	567/2	2,2,2	-3375/16
2,2,1,1	6075/16	2,1,1,1,1	-1215/16	1,1,1,1,1,1	243/80
7	-49149/7	6,1	49140/8	5,2	36828/8
5,1,1	-27621/10	4,3	32130/8	4,2,1	-34425/8
4,1,1,1	6885/8	3,3,1	-15876/8	3,2,2	-14175/8
3,2,1,1	17010/8	3,1,1,1,1	-1701/8	2,2,2,1	10125/16
2,2,1,1,1	-6075/16	2,1,1,1,1,1	729/16	1,1,1,1,1,1,1	-729/560
8	-1376235/56	7,1	1179576/56	6,2	859950/56
6,1,1	-515970/56	5,3	902286/70	5,2,1	-773388/56
5,1,1,1	193347/70	4,4	390150/64	4,3,1	-674730/56
4,2,2	-344250/64	4,2,1,1	413100/64	4,1,1,1,1	-41310/64
3,3,2	-277830/56	3,3,1,1	166698/56	3,2,2,1	297675/56
3,2,1,1,1	-119070/56	3,1,1,1,1,1	10206/80	2,2,2,2	50625/128
2,2,2,1,1	-60750/64	2,2,1,1,1,1	18225/64	2,1,1,1,1,1,1	-1458/64
1,1,1,1,1,1,1,1	2187/4480				

Table 3.2. Alpha coefficients found by PSLQ computations.

Next, from the above results, one can immediately read that $\alpha([]) = 3$, $\alpha([1]) = -9$, $\alpha([2]) = -45/2$, $\alpha([1,1]) = 27/2$, and so forth. Table 3.6 presents the values of α that we obtained in this manner.

Using these values, we then calculated series approximations to the functions $P_k(x)$, by using formula (3.34). We obtained

$$\begin{aligned}
P_3(x) &\approx 3 - \frac{45}{4}x^2 - \frac{45}{16}x^4 - \frac{45}{64}x^6 - \frac{45}{256}x^8 - \frac{45}{1024}x^{10} - \frac{45}{4096}x^{12}x^{14} \\
&\quad - \frac{45}{16384} - \frac{45}{65536}x^{16}, \\
P_4(x) &\approx 3 - \frac{49}{4}x^2 + \frac{119}{144}x^4 + \frac{3311}{5184}x^4 + \frac{38759}{186624}x^6 + \frac{384671}{6718464}x^8 \\
&\quad + \frac{3605399}{241864704}x^{10} + \frac{33022031}{8707129344}x^{12} + \frac{299492039}{313456656384}x^{14}, \\
P_5(x) &\approx 3 - \frac{205}{16}x^2 + \frac{7115}{2304}x^4 + \frac{207395}{331776}x^6 + \frac{4160315}{47775744}x^8 \\
&\quad + \frac{74142995}{6879707136}x^{10} + \frac{1254489515}{990677827584}x^{12} \\
&\quad + \frac{20685646595}{142657607172096}x^{14} + \frac{336494674715}{20542695432781824}x^{16}, \\
P_6(x) &\approx 3 - \frac{5269}{400}x^2 + \frac{6640139}{1440000}x^4 + \frac{1635326891}{5184000000}x^6 \\
&\quad - \frac{5944880821}{18662400000000}x^8 - \frac{212874252291349}{67184640000000000}x^{10} \\
&\quad - \frac{141436384956907381}{241864704000000000000}x^{12} \\
&\quad - \frac{70524260274859115989}{870712934400000000000000}x^{14} \\
&\quad - \frac{31533457168819214655541}{3134566563840000000000000000}x^{16}, \\
P_7(x) &\approx 3 - \frac{5369}{400}x^2 + \frac{8210839}{1440000}x^4 - \frac{199644809}{5184000000}x^6 \\
&\quad - \frac{680040118121}{18662400000000}x^8 - \frac{278500311775049}{67184640000000000}x^{10} \\
&\quad - \frac{84136715217872681}{241864704000000000000}x^{12}
\end{aligned}$$

$$- \frac{22363377813883431689}{870712934400000000000000} x^{14}$$
$$- \frac{55600908402639114288841}{31345665638400000000000000} x^{16}.$$

With these approximations in hand, we were then in a position to attempt to determine closed-form expressions for $P_k(x)$. This can be done by using the `Pade` function in either *Mathematica* or *Maple*. We obtained the following:

$$\begin{aligned}
P_1(x) &\stackrel{?}{=} 3, \\
P_2(x) &\stackrel{?}{=} \frac{3(4x^2-1)}{(x^2-1)}, \\
P_3(x) &\stackrel{?}{=} \frac{12(4x^2-1)}{(x^2-4)}, \\
P_4(x) &\stackrel{?}{=} \frac{12(4x^2-1)(4x^2-9)}{(x^2-4)(x^2-9)}, \\
P_5(x) &\stackrel{?}{=} \frac{48(4x^2-1)(4x^2-9)}{(x^2-9)(x^2-16)}, \\
P_6(x) &\stackrel{?}{=} \frac{48(4x^2-1)(4x^2-9)(4x^2-25)}{(x^2-9)(x^2-16)(x^2-25)}, \\
P_7(x) &\stackrel{?}{=} \frac{192(4x^2-1)(4x^2-9)(4x^2-25)}{(x^2-16)(x^2-25)(x^2-36)}.
\end{aligned}$$

These results immediately suggest that the general form of a generating function identity is

$$\sum_{n=0}^{\infty} \zeta(2n+2)x^{2n} \stackrel{?}{=} 3 \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}(k^2-x^2)} \prod_{m=1}^{k-1} \frac{4x^2-m^2}{x^2-m^2}, \tag{3.40}$$

which is equivalent to (3.30).

We next confirmed this result in several ways:

1. We symbolically computed the power series coefficients of the left-hand side and the right-hand side of (3.40), and have verified that they agree up to the term with x^{100}.

2. We verified that $\mathscr{Z}(1/6)$, where $\mathscr{Z}(x)$ is the RHS of (3.40), agrees with $18 - 3\sqrt{3}\pi$, computed using (3.31), to over 2,500 digit precision; likewise for $\mathscr{Z}(1/2) = 2$, $\mathscr{Z}(1/3) = 9/2 - 3\pi/(2\sqrt{3})$, $\mathscr{Z}(1/4) = 8 - 2\pi$, and $\mathscr{Z}(1/\sqrt{2}) = 1 - \pi/\sqrt{2} \cdot \cot(\pi/\sqrt{2})$.

3. We then affirmed that the formula (3.40) gives the same numerical value as (3.31) for the 100 pseudorandom values $\{m\pi\}$, for $1 \leq m \leq 100$, where $\{\cdot\}$ denotes fractional part.

Thus, we were certain that (3.30) was correct, and it remained only to find a proof of Theorem 3.4. This can been done by applying the Wilf-Zeilberger method. See [16] for details.

4 Exploration and Discovery in Inverse Scattering

> Today a single computer can do more arithmetic operations in a year, than all of mankind has done from its beginnings till 1945 when the first electronic computer became operational. ...this achievement is insignificant when measured against the vastness of what one might call the "mathematical universe."
>
> —Hans J. Bremermann [74]

4.1 Metaphysics and Mechanics

The mathematical study of physical processes is conventionally split between modeling and, once the modeling is sufficiently mature, manipulation and data analysis. The modeling stage of exploration has a natural experimental component that conforms to the usual picture conjured by the word *experiment*, that is, a laboratory with machines that funnel physical processes through a narrowly defined, well controlled environment for the purpose of isolating and observing phenomena. Here mathematics serves as a language to describe physical processes and to focus rational exploration.

In this chapter, we focus on the data analysis side of experimental mathematics, and, as such, we take the models for granted. Indeed, we make no distinction between the models and the physical processes they describe. We are interested instead in the inverse problem of determining the model from an observation.

Inverse problems are not new to applied mathematics. The inverse scattering techniques we detail below, however, are still in their infancy and point to a shifting approach to inverse problems in general which we would like to take a moment to contrast with more conventional methodologies. Statistical regression and estimation, for instance, have long been fundamental to empirical studies that seek to find the most likely model to fit some observed data. Here the model for the data is given a priori with undetermined parameters that are selected by an optimization procedure which yields a best fit to the observation according to some criteria, often depending on an assumed noise or stochastic model. Quantitative confidence intervals can be obtained that provide bounds on the likelihood that a given model assumption is true, through a procedure known as *hypothesis testing*.

This process of quantitatively deducing a likely explanation for an observation fits very naturally in the mold of experimental mathematics and could easily be considered the template for experimental mathematics as it is applied elsewhere. What distinguishes conventional inverse problems from the case study presented here is the amount of a priori information we allow ourselves and the nature of the information we glean from our mathematical experiments. We assume relatively little at the outset about the model for the data and, through a series of qualitative feasibility tests, progressively refine our assumptions. The feasibility tests are Boolean in nature—very much in the spirit of a yes/no query to an oracle that is constructed from the governing equations. As certain possibilities are ruled out, we can then begin the process of obtaining quantitative estimates for specific parameters. At the final stages of the process our techniques will merge with conventional parameter estimation techniques, but it is the process of getting to that stage of refinement that is of recent vintage and a topic of current research.

Another reason for placing the spotlight on inverse scattering is to highlight the role of computational experimentation in the development of mathematical methodologies. The settings in which the methods we explore can be mathematically proven to work are far fewer than those in which they have been computationally demonstrated to work. At the same time, uniqueness proofs for the solutions to boundary value problems in partial differential equations have been the motivation for many computational techniques. This interplay between computation and theory is central to experimental mathematics.

The following is a case study of recent trends in *qualitative* exploration of the mathematical structure of models for the scattering of waves and their corresponding inverse operators. This approach has its roots in functional analysis methods in partial differential equations and has merged with engineering and numerical analysis. Applications range from acoustic scattering for geophysical exploration to electromagnetic scattering for medical imaging. As the mathematical models for acoustic and electromagnetic scattering share identical formulations in many instances, it follows that the methods we describe below apply to both electromagnetic and acoustic scattering. For ease, however, our case study is for acoustic scattering.

4.2 The Physical Experiment

The experiment consists of sending a wave through a domain $\mathbb{D} \subset \mathbb{R}^2$ containing, for the most part, homogeneous isotropic material. What we are looking for is small, relative to the domain $\mathbb{D}$, inhomogeneities inside this domain. The inhomogeneities, also called *scatterers*, will be referred to both by the functional description of the inhomogeneity, what we define below as the *scattering potential*, $m : \mathbb{R}^2 \to \mathbb{R}$, and by the interior of the support of the scattering potential, $\Omega \equiv \text{int}(\text{supp}(m))$.

Most of our readers will be familiar with the joke about a physicist who, upon explaining his proposed solution to increasing milk production in cows, begins with, "First, let us assume a spherical cow." In that spirit, when we pass from the physical experiment to the mathematical model in Section 4.3, we will consider the domain $\mathbb{D}$ to be a ball of infinite radius the boundary of which is parameterized by the directions $\widehat{x}$ on the unit sphere, which we denote by $\mathbb{S} \equiv \{\widehat{x} \in \mathbb{R}^2 \mid |\widehat{x}| = 1\}$.

To fix this idea firmly, imagine that a doctor wraps a patient with a belt of ultrasonic transducers and receivers. The domain $\mathbb{D}$ is the cross-section of the (cylindrical) human torso through which a doctor sends ultrasonic waves and records the resulting field on the skin of this cross section of the torso—certainly preferable to making measurements *inside* the body! Relative to the wavelength of the ultrasonic wave (typically 0.3–1.54 mm) the torso (typically 100–250 mm in radius) is a very large domain—practically infinite.

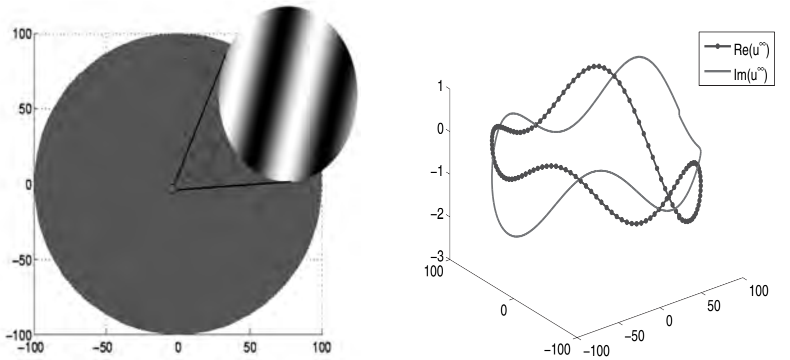
The illuminating wave is a small amplitude, monochromatic, time-harmonic acoustic plane wave denoted

$$u^i(x; \widehat{\eta}, \kappa) \equiv e^{i\kappa\widehat{\eta}\cdot x}, \quad x \in \mathbb{R}^2, \tag{4.1}$$

and parameterized by the incident direction $\widehat{\eta}$ in the set $\mathbb{S}$ of unit vectors in $\mathbb{R}^2$ and wavenumber $\kappa > 0$. What is recorded is the resulting *far field pattern* for the scattered field, denoted by $u^\infty(\cdot, \widehat{\eta}, \kappa) : \partial\mathbb{D} \to \mathbb{C}$ at points $\widehat{x}$ uniformly distributed around $\partial\mathbb{D}$, the boundary of $\mathbb{D}$. By "far field" we mean that the radius of $\mathbb{D}$ is large relative to the wavelength and that whatever is causing the scattering lies well inside the interior of $\mathbb{D}$. The incident field with wavenumber $\kappa = 2$ at points $x \in \mathbb{D}$, a circle of radius 100 centered at the origin, and the resulting far field pattern are shown in Figure 4.1. The restriction to two-dimensional space is a matter of computational convenience—the theory applies equally to $\mathbb{R}^3$. The length scales are determined by κ which is inversely proportional to the wavelength, $\omega = 2\pi/\kappa$ *physical units*.

The time-dependence of the wave has already been factored out since the time-harmonicity only contributes an $e^{-i\omega t}$ factor to the waves. The isotropy assumption on the domain $\mathbb{D}$ means that there is no preferential direction of scattering. This is not the same as assuming that there are no obstructions to the wave since, otherwise, the far field pattern would be zero.

Since our experiments are at a single fixed frequency, $\kappa = 2$, we shall drop the explicit dependence of the fields on κ. The representation of the fields as mappings onto $\mathbb{C}$ is also, to some degree, a matter of convenience. For acoustic



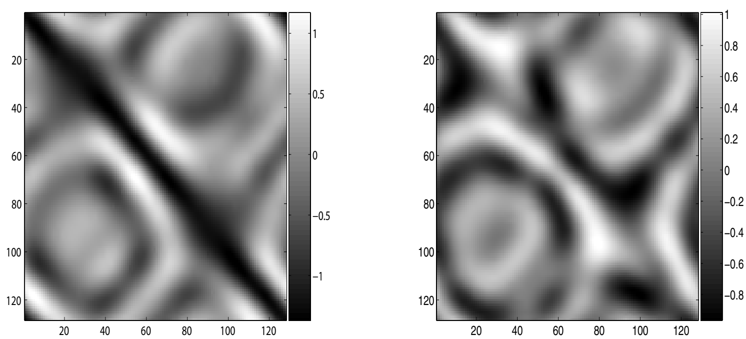
(a) (b)

Figure 4.1. (a) Real part of incident field with direction $\widehat{\eta} = -\pi/12$, and wavenumber $\kappa = 2$ on the domain $\mathbb{D}$. The inset is a close-up view of the field. (b) Far field data, real and imaginary parts, corresponding to scattering due to the passing of the incident plane wave shown in (a) through the domain $\mathbb{D}$.

experiments it is possible to measure the *phase* of the fields, that is, the real and imaginary parts. This is not always the case for electromagnetic experiments [204], though we avoid these complications.

The experiment is repeated at N incident directions $\widehat{\eta}_n$ equally distributed on the interval $[-\pi, \pi]$. For each incident direction $\widehat{\eta}_n$, we collect N far field measurements at points $\widehat{x}_n$. The resulting arrays of data are $N \times N$ complex-valued matrices shown in Figure 4.2.

Our goal is to determine as much as possible about the scatterer(s) that produced this data. We will be satisfied with being able to locate and determine the



(a) (b)

Figure 4.2. Far field data, real (a) and imaginary (b) parts, from a series of acoustic scattering experiments differing in the direction of the incident field. Each experiment is at the same incident wavenumber $\kappa = 2$.

size and shape of the scatterers. If we can determine some of the physical properties of the material making up the scatterers, we will be at the cutting edge of inverse scattering research. We begin with a review of acoustic scattering. This theory is classical, hence our treatment is terse. Readers interested in thorough derivations of the tools we explore are referred to [98] from which we borrow our formalism.

4.3 The Model

Our a priori knowledge is limited to the incident waves u^i and the *background medium* in $\mathbb{D}$, namely that they are small-amplitude, monochromatic plane waves traveling in an isotropic medium. The waves travel in space and as such are represented as vector-valued functions of their position. Since the medium is isotropic, however, the vector components of the wave fields are not coupled, thus we can treat each of the spatial components of the wave as independent scalar waves obeying the same governing equations. As mentioned above, if there were no obstructions to u^i in $\mathbb{D}$, the far field pattern would be zero. As this is apparently not the case, there must be some *scattered field*, which we denote by u^s, generated by the interaction of u^i with a *scatterer*. We describe the scatterer in more detail below. Together the scattered field and the incident field comprise the *total field*, denoted u, where

$$u(x,\widehat{\eta}) = u^i(x,\widehat{\eta}) + u^s(x,\widehat{\eta}). \tag{4.2}$$

For slowly varying scatterers, the governing equations for acoustic scattering are given by

$$\left(\triangle + n(x)\kappa^2\right) u(x) = 0, \quad x \in \mathbb{R}^2, \tag{4.3}$$

where $\triangle$ denotes the Laplacian and $n : \mathbb{R}^2 \to \mathbb{C}$ is the *index of refraction of the medium*. Note that the incident plane wave u^i satisfies the *Helmholtz equation*, that is, (4.3) with $n(x) \equiv 1$. In terms of the speed of propagation through the medium, this is given by

$$n(x) := \frac{c_0^2}{c^2(x)} + i\sigma(x), \tag{4.4}$$

where $c_0 > 0$ denotes the sound speed of the background medium, $c : \mathbb{R}^2 \to \mathbb{R}_+ \setminus \{0\}$ is the sound speed inside the scatterer, and $\sigma : \mathbb{R}^2 \to \mathbb{R}_+$ is a function that models the influence of absorption. Note that, at a point x in the background medium, $\frac{c_0^2}{c^2(x)} = 1$. We assume that the background medium is nonabsorbing, that is, $\sigma(x) = 0$, hence $n(x) = 1$ in the background medium. For what follows, it is more convenient to work with the *scattering potential*, defined by

$$m \equiv 1 - n. \tag{4.5}$$

Note that from the assumptions above $m(x) = 0$ in the background medium. Moreover, we assume that m has compact support. The slowly varying assumption means that derivatives of the index of refraction, or equivalently the scattering potential, of order 1 and higher are well defined and negligible, though the threshold to negligibility can be quite high.

We will frequently refer to the scatterer as those points where the scattering potential is nonzero:

$$\Omega \equiv \left\{ x \in \mathbb{R}^2 \mid m(x) \neq 0 \right\}, \qquad \Omega^o \equiv \mathbb{R}^2 \setminus \overline{\Omega}, \tag{4.6}$$

where $\overline{\Omega}$ denotes the closure of the (open) scattering domain Ω. If the scatterer is a sound reflector ($c^2(x) \ll 1$) or a highly absorbing material ($\sigma \gg 1$) (or some combination of these), then we restrict the domain in (4.3) from $\mathbb{R}^2$ to the open exterior domain Ω^o. The scatterers are then modeled as *obstacles* that behave as either *sound soft* or *sound hard* obstacles, or some mixture of these. This is modeled with Dirichlet, Neumann, or Robin boundary conditions on $\partial\Omega$,

$$u = f \quad \text{or} \quad \frac{\partial u}{\partial \nu} = f \quad \text{or} \quad \frac{\partial u}{\partial \nu} + \lambda u \; = \; f \quad \text{on } \partial\Omega, \tag{4.7}$$

where f is continuous on $\partial\Omega$, ν is the unit outward normal, and λ is an *impedance function*.

In either case, slowly varying media or obstacle scattering, the scattered field u^s is a decaying field satisfying what is known as the *Sommerfeld radiation condition*,

$$r^{\frac{1}{2}} \left(\frac{\partial}{\partial r} - i\kappa \right) u^s(x) \to 0, \;\; r = |x| \to \infty, \tag{4.8}$$

uniformly in all directions. Solutions to the Helmholtz equation that satisfy (4.8) are also called *radiating* solutions to the Helmholtz equation.

We prefer the formulation as slowly varying media to obstacle scattering since the latter can be viewed as an ideal limiting case of the former. If, in the course of our investigation it appears that there is some obstacle scattering present, we can always refocus our investigation to take this into account.

For inhomogeneous media, the far field pattern—what is actually measured—is modeled by the leading term in the asymptotic expansion for u^s as $|x| \to \infty$, namely

$$u^s(x, \widehat{\eta}) = \beta \frac{e^{i\kappa|x|}}{|x|^{1/2}} u^\infty(\widehat{x}, \widehat{\eta}) + o\left(\frac{1}{|x|^{1/2}} \right), \qquad \widehat{x} = \frac{x}{|x|}, \tag{4.9}$$

where

$$\beta = \left(\frac{e^{i\frac{\pi}{2}}}{8\pi\kappa}\right)^{1/2} \tag{4.10}$$

and

$$u^\infty(\widehat{x},\widehat{\eta}) \equiv -\kappa^2 \int_{\mathbb{R}^2} e^{-i\kappa y\cdot\widehat{x}} m(y)u(y,\widehat{\eta})\, dy. \tag{4.11}$$

In an abuse of notation we have replaced points $\widehat{x} \in \partial\mathbb{D}$ with directions on the unit sphere $\widehat{x} \in \mathbb{S} \equiv \left\{\widehat{x} \in \mathbb{R}^2 \mid |\widehat{x}| = 1\right\}$, which is tantamount to letting $\partial\mathbb{D} \to \infty$ in all directions, consistent with the asymptotic expression for u^∞. Until we return to the realm of the real world in numerical implementations, we replace the experimental domain $\mathbb{D}$ with all of $\mathbb{R}^2$, the boundary of which is the set of directions $\mathbb{S}$.

Though the model above was developed for incident plane waves $u^i(x,\widehat{\eta}) = e^{i\kappa\widehat{\eta}\cdot x}$, it holds equally well for any generic incident wave v^i that satisfies the Helmholtz equation ((4.3) with $n(x) \equiv 1$) with u, u^s, and u^∞ in (4.2)–(4.11) replaced by the respective generic total, scattered, and far fields v, v^s, and v^∞. We are now in a position to state the fundamental problem of scattering:

> Given a slowly varying index of refraction n defined by (4.4) that is different than 1 only on the interior of some ball, and an incident field v^i satisfying the Helmholtz equation everywhere, the *scattering problem* is to find v that satisfies (4.3) and $v = v^i + v^s$, where v^s satisfies the Sommerfeld Radiation Condition (4.8) uniformly in all directions.
>
> Given v^i and partial information about v^∞ defined by (4.11), the *inverse scattering problem* is to determine *anything* about the scattering potential $m = 1 - n$.

Since we will be trying to reconstruct volumetric information from boundary measurements, it shouldn't come as a surprise that a central tool in our analysis is Green's theorem: For an arbitrary bounded domain $\mathbb{V}$ with C^2 (twice differentiable[1]) boundary

$$\int_{\mathbb{V}} (v\triangle u + \nabla v\cdot\nabla u)\, dx = \int_{\partial\mathbb{V}} v\frac{\partial u}{\partial\nu}\, ds \tag{4.12}$$

for $u \in C^2(\overline{\mathbb{V}})$ and $v \in \mathbb{C}^1(\overline{\mathbb{V}})$, the unit outward normal to $\mathbb{V}$, ν. For $v \in \mathbb{C}^2(\overline{\mathbb{V}})$ Green's second theorem is

$$\int_{\mathbb{V}} (v\triangle u - u\triangle v)\, dx = \int_{\partial\mathbb{V}} v\frac{\partial u}{\partial\nu} - u\frac{\partial v}{\partial\nu}\, ds. \tag{4.13}$$

[1]Green's theorem only requires a C^1 boundary, but we will need a C^2 boundary for Green's formula next.

We will also make use of Green's formula: For $v \in C^2(\mathbb{V}) \cap C(\overline{\mathbb{V}})$ that possesses a normal derivative on $\partial\mathbb{V}$,

$$\begin{aligned} v(x) &= \int_{\partial\mathbb{V}} \left(\Phi(x,y)\frac{\partial v}{\partial \nu}(y) - v(y)\frac{\partial \Phi(x,y)}{\partial \nu(y)} \right) ds(y) \\ &\quad - \int_{\mathbb{V}} \left(\triangle v(y) + \kappa^2 v(y)\right) \Phi(x,y)\, dy, \quad x \in \mathbb{V}. \end{aligned} \tag{4.14}$$

Here $\Phi(\cdot, y) : \mathbb{R}^2 \setminus \{y\} \to \mathbb{C}$ is the free space (no scatterer) radiating (that is, it satisfies (4.8)) fundamental solution to (4.3),

$$\Phi(x,y) := \frac{i}{4} H_0^{(1)}(\kappa|x-y|), \qquad x \neq y, \tag{4.15}$$

with $H_0^{(1)}$ denoting the zeroth order Hankel function of the first kind.

For smooth boundaries $\partial\Omega$, (4.9), (4.14), and the asymptotic expansion of Φ with respect to $|x|$ yield

$$u^\infty(\widehat{x}, \widehat{\eta}) = \beta \int_{\partial\Omega} \left(u^s(y, \widehat{\eta}) \frac{\partial e^{-i\kappa \widehat{x}\cdot y}}{\partial \nu(y)} - \frac{\partial u^s(y, \widehat{\eta})}{\partial \nu} e^{-i\kappa \widehat{x}\cdot y} \right), \quad \widehat{x}, \widehat{\eta} \in \mathbb{S}. \tag{4.16}$$

Here we have used the fact that u^s satisfies (4.8) and the Helmholtz equation ((4.3) with $n \equiv 1$) on the domain $\mathbb{V}$ with interior boundary $\partial\Omega$ and exterior boundary $\lim_{r\to\infty} r\mathbb{S}$—which is why the second part of (4.14) is missing from the above expression. Moreover, it can be shown that the far field due to an incident plane wave enjoys a symmetry

$$u^\infty(\widehat{x}, \widehat{\eta}) = u^\infty(-\widehat{\eta}, -\widehat{x}\,). \tag{4.17}$$

This relation is the well-known *reciprocity* relation for the far field.

A very useful tool in our analysis and algorithms are fields that can be represented as the superposition of plane waves. Define the *Herglotz wave operator* $\mathscr{H} : L^2(\mathbb{S}) \to L^2(\mathbb{R}^2)$ by

$$(\mathscr{H} g)(x) \equiv \int_{\mathbb{S}} e^{i\kappa x\cdot(-\widehat{y}\,)} g(-\widehat{y}\,) ds(\widehat{y}), \quad x \in \mathbb{R}^2. \tag{4.18}$$

Corresponding to the Herglotz wave operator is the *Herglotz wave function*, which we denote by $v_g^i \equiv (\mathscr{H} g)(x)$. If we can write some generic incident field v^i as a Herglotz wave function, that is, $v^i \to v_g^i$ is a superposition of plane waves weighted by $g \in L^2(\mathbb{S})$, then v_g^i is an entire solution to the Helmholtz equation, and the corresponding scattered and far fields have analogous expressions [244]:

$$v_g^s(x) \;=\; \int_{\mathbb{S}} u^s(x, -\widehat{\eta}) g(-\widehat{\eta}) ds(\widehat{\eta}) \tag{4.19}$$

and

$$v_g^\infty(\widehat{x}) = \int_{\mathbb{S}} u^\infty(\widehat{x}, -\widehat{\eta}) g(-\widehat{\eta}) ds(\widehat{\eta}), \qquad \widehat{x} \in \mathbb{S}. \tag{4.20}$$

Note that (4.19) satisfies (4.8) and $v_g = v_g^i + v_g^s$ is a solution to the scattering problem.

Remark 4.1. The signs in the expressions for v_g^i, v_g^s, and v_g^∞ above have been chosen so that the backpropagation mapping between the far field measurements and the scattered field, which we derive later, has a natural interpretation in terms of a physical aperture in the far field. The development given here is for *full aperture* measurements, that is, u^∞ is measured on the entire far field sphere. The first of the methods discussed below also holds for *limited aperture* settings where the far field is measured on an open subset $\mathbb{S}'$ of the far field sphere $\mathbb{S}$. In this case, the function g is defined on $-\mathbb{S}'$, the mirror image of the interval $\mathbb{S}'$: $\widehat{\eta} \in \mathbb{S}' \subset \mathbb{S} \iff -\widehat{\eta} \in -\mathbb{S}'$. Using the far field reciprocity relation (4.17) we see that the far field is defined on $\mathbb{S}'$ with any incident wave direction $-\widehat{x}$:

$$v_g^\infty(\widehat{x}) = \int_{\mathbb{S}'} u^\infty(\widehat{\eta}, -\widehat{x}) g(-\widehat{\eta}) ds(\widehat{\eta}), \qquad \widehat{x} \in \mathbb{S}. \tag{4.21}$$

It is worthwhile taking a second look at the Herglotz wave operator (4.18). This operator, restricted to L^2 functions on the boundary of some domain $\Omega_t \subset \mathbb{R}^m$ with piecewise C^2 boundary and connected exterior, is *almost always*[2] injective with dense range [99]. In particular, we can construct the density $g(\cdot; z)$ such that $v^i_{g(\cdot,z)}(x) \approx \Phi(x,z)$ and

$$\frac{\partial v^i_{g(\cdot,z)}}{\partial n}(x) \approx \frac{\partial \Phi(x,z)}{\partial n}$$

arbitrarily closely for $x \in \partial\Omega$ and $z \in \Omega^o$. By (4.14) and (4.20), for $z \in \Omega^o$ and any generic scattered field u^s satisfying the Helmholtz equation and the radiation condition (4.8), we have

$$\begin{aligned} u^s(z) &= \int_{\partial\Omega} \left\{ \Phi(y,z) \frac{\partial u^s}{\partial \nu}(y) - \frac{\partial \Phi(y,z)}{\partial \nu(y)} u^s(y) \right\} ds(y) \\ &\approx \int_{\partial\Omega} \left\{ v^i_{g(\cdot;z)}(y) \frac{\partial u^s}{\partial \nu}(y) - \frac{\partial v^i_{g(\cdot;z)}(y)}{\partial \nu(y)} u^s(y) \right\} ds(y) \end{aligned}$$

[2]The reason for the *almost always* caveat is that the Herglotz wave operator is not injective if the interior homogeneous Dirichlet problem on Ω_t (that is, the Helmholtz equation on this domain with Dirichlet boundary values) has nontrivial solutions. If this is the case, then the wavenumber κ is an *eigenvalue* for this problem. But, fortunately, the set of eigenvalues is countable, hence the *almost always* caveat.

$$= \int_{\mathbb{S}}\int_{\partial\Omega}\left\{e^{i\kappa y\cdot(-\widehat{x})}\frac{\partial u^s}{\partial\nu}(y) - \frac{\partial e^{i\kappa y\cdot(-\widehat{x})}}{\partial\nu(y)}u^s(y)\right\}ds(y)g(-\widehat{y};z)ds(\widehat{y})$$

$$= \int_{\mathbb{S}} u^\infty(\widehat{y})g(-\widehat{y};z)ds(\widehat{y}). \tag{4.22}$$

In moving from the second line to the third of this approximation, we replaced v_g^i with its integral representation and switched the order of integration.

There are two ways to view this last integral that distinguishes many numerical methods in inverse scattering. By the first interpretation the last integral in (4.22) is an integral operator with the far field pattern u^∞ as a kernel. When the scattering is from an incident plane wave, this operator is called the *far field operator* $\mathscr{F}$: $L^2(\mathbb{S}) \to L^2(\mathbb{S})$,

$$\mathscr{F} f(\widehat{x}) \equiv \int_{\mathbb{S}} u^\infty(\widehat{\eta},\widehat{x})f(-\widehat{\eta})\; ds(\widehat{\eta}). \tag{4.23}$$

The fact that $(\mathscr{F} g(\cdot;z))(\widehat{x}) \approx u^s(z,\widehat{x})$ is a happy circumstance of having selected the correct function g to operate on. By the second interpretation the last integral in (4.22) is an integral operator with the density $g(\cdot;z)$ as a kernel: $\mathscr{A} : L^2(\mathbb{S}) \to \mathbb{X}(z)$,

$$\mathscr{A} f(z) \equiv \int_{\mathbb{S}} g(-\widehat{\eta};z)f(\widehat{\eta})\; ds(\widehat{\eta}). \tag{4.24}$$

Since the image space of this operator depends on *how* the density g is constructed pointwise (a detail we will only briefly touch upon here), we indicate this ambiguity by denoting the image space with the as-yet-to-be-determined space $\mathbb{X}$. Acting on the far field pattern corresponding to an incident plane wave with direction $\widehat{x}$, the operator $\mathscr{A}$ can be seen to be a *backpropagation operator* that propagates the far field back to the scattered field at $z \in \Omega^o$. We will occupy ourselves mostly with the former interpretation.

4.3.1 Integral Equation Formulation

The scattering model is conventionally reformulated as an integral equation, which admits both existence and uniqueness theorems as well as numerical algorithms. To do this we make use of the *volume potential*

$$(\mathscr{V}\varphi)(x) \equiv \int_{\mathbb{R}^m} \Phi(x,y)m(y)\varphi(y)\; dy, \;\; x \in \mathbb{R}^2, \tag{4.25}$$

where m is the scattering potential (4.5). If u satisfies (4.2), (4.3), and (4.8) and is twice continuously differentiable on $\mathbb{R}^2$, i.e., $u \in C^2(\mathbb{R}^2)$, then by (4.14) applied to u we have

$$u(x) = \int_{\partial r\mathbb{B}} \left(\frac{\partial u}{\partial \nu} \Phi(x,y) - u(y) \frac{\partial \Phi(\cdot, y)}{\partial \nu(y)}(x) \right) ds(y)$$
$$-\kappa^2 \int_{r\mathbb{B}} \Phi(x,y) m(y) u(y)\, dy, \tag{4.26}$$

where $r\mathbb{B}$ is the ball of radius r with $\operatorname{supp}(m) \in \operatorname{int}(r\mathbb{B})$ and $x \in \operatorname{int}(r\mathbb{B})$ and ν is the unit outward normal to $r\mathbb{B}$. Here we have used the fact that u satisfies (4.3) and $m = 1 - n$. Applying (4.14) to the incident field u^i yields

$$u^i(x) = \int_{\partial r\mathbb{B}} \left(\frac{\partial u^i}{\partial \nu} \Phi(x,y) - u^i(y) \frac{\partial \Phi(\cdot, y)}{\partial \nu(y)}(x) \right) ds(y). \tag{4.27}$$

Moreover, (4.12) applied to u^s together with the boundary condition (4.8) gives

$$0 = \int_{\partial r\mathbb{B}} \left(\frac{\partial u^s}{\partial \nu} \Phi(x,y) - u^s(y) \frac{\partial \Phi(\cdot, y)}{\partial \nu(y)}(x) \right) ds(y). \tag{4.28}$$

Altogether, (4.26)–(4.28) and (4.2) yield the well-known *Lippmann-Schwinger* integral equation

$$u = u^i - \kappa^2 \mathscr{V} u. \tag{4.29}$$

From (4.2) it follows immediately from (4.29) that

$$u^s(x, \widehat{\eta}) = -\kappa^2 (\mathscr{V} u)(x, \widehat{\eta}). \tag{4.30}$$

With a little more work [98, Theorem 8.1 and 8.2] it can be shown that if $u \in C(\mathbb{R}^2)$ solves (4.29), then u satisfies (4.2)–(4.8) for $n \in C^1(\mathbb{R}^2)$. We summarize this discussion with the following well-known fact.

Theorem 4.2 (Helmholtz-Lippmann-Schwinger Equivalence). *If $u \in C^2(\mathbb{R}^2)$ satisfies (4.2)–(4.8) for $n \in C^1(\mathbb{R}^2)$, then u solves (4.29). Conversely, if $u \in C^2(\mathbb{R}^2)$ solves (4.29), then u solves (4.2)–(4.8).*

The previous theorem assumed that the solutions to (4.2)–(4.8) and equivalently (4.29) exist, which begs the question about existence and uniqueness.

Theorem 4.3. *For each $\kappa > 0$ there exists a unique u satisfying (4.2), (4.3), and (4.8) with u^i given by (4.1). Moreover, u depends continuously on u^i with respect to the max-norm.*

Proof sketch: The main ideas are sketched here. Interested readers are referred to the works of Leis [196], Reed and Simon [246], and Colton and Kress [98]. The integral operator $\mathscr{V}$ has a weakly singular kernel Φ, hence is a compact operator $C(\overline{\mathbb{V}}) \to C(\overline{\mathbb{V}})$ where $\Omega \in \operatorname{int}(\mathbb{V})$ for $\mathbb{V}$ bounded. Standard results in integral equations [187,249] ensure that, if the homogeneous Lippmann-Schwinger equation

$$u + \kappa^2 \mathscr{V} u = 0,$$

has only the trivial solution, then the inhomogeneous equation has a unique solution and the inverse operator $(I + \kappa^2 \mathscr{V})^{-1}$ exists and is bounded in $C(\overline{\mathbb{V}})$. Since the inverse operator is bounded, the solution u depends continuously on u^i with respect to the max-norm on $C(\overline{\mathbb{V}})$. From the previous discussion, the homogeneous Lippmann-Schwinger equation is equivalent to

$$\left(\triangle + n(x)\kappa^2\right) u(x) = 0, \quad x \in \mathbb{R}^2, \tag{4.31}$$

and

$$r^{\frac{1}{2}} \left(\frac{\partial}{\partial r} - i\kappa\right) u(x) \to 0, \;\; r = |x| \to \infty. \tag{4.32}$$

Green's Theorem (4.12) and the unique continuation principle [196] are employed to show that the only solution to (4.31)–(4.32) is the trivial solution. □

The natural question to ask next is *what* about the index of refraction n is encoded in the far field data u^∞. This is the central question in inverse scattering and one that often leads to algorithms. In the next section we shall motivate some representative inverse scattering algorithms by the uniqueness results at their foundation.

4.4 The Mathematical Experiment: Qualitative Inverse Scattering

In the previous sections we established the geometry and basic mathematical model detailed in the present section—to pick up on an earlier reference, we approximated a cow by a sphere. There is another joke between physicists and mathematicians that is pertinent: Physicists make simple observations about complicated things while mathematicians make complicated observations about simple things. There is a lot of truth to the statement, and it will certainly apply here. However, an investigation of the mathematical properties of the model described in the previous sections is essential to discovering how to get information out of even the simplest physical devices without sacrificing our spherical cow. From the lay person's perspective, the object is to replace biopsy by some painless, noninvasive imaging technology like CT, MRI, or ultrasound. From the mathematician's perspective, it starts with the theory of partial differential equations.

A long standing problem has been to determine when the scattering potential is uniquely determined by the far field. The answer to this question is subtle and varied, depending on the setting—whether $\mathbb{R}^2$ or $\mathbb{R}^3$, isotropic or anisotropic, multi-frequency or single frequency, Dirichlet, Neumann, or inhomogeneous media. In three or more dimensions for isotropic media, key results affirming the recovery of $n(x)$ from $u^\infty(\widehat{x};\widehat{\eta})$, where u^∞ is known for all $\widehat{x},\widehat{\eta} \in \mathbb{S}$, can be found in Nachman [218], Novikov [221], and Ramm [244]. In two dimensions, the case we consider here, positive results are more difficult. A quick heuristic as to why this might be the case is to look at the dimensions of the data versus those of the unknown index of refraction n. In $\mathbb{R}^3$ the dimension of $n : \mathbb{R}^3 \to \mathbb{C}$ is three while the data $u^\infty : \mathbb{S} \times \mathbb{S} \to \mathbb{C}$ is on two two-dimensional spheres, $\widehat{x} \in \mathbb{S}$ and $\widehat{\eta} \in \mathbb{S}$, so that the problem appears to be overdetermined. By contrast, in $\mathbb{R}^2$ the unknown $n : \mathbb{R}^2 \to \mathbb{C}$ and the data $u^\infty : \mathbb{S} \times \mathbb{S} \to$ are both two-dimensional since, in this case, the spheres $\mathbb{S}$ are one-dimensional. The same *kind* of data in $\mathbb{R}^2$ does not stretch as far is it does in $\mathbb{R}^3$.

Two-dimensional results for *small* potentials are given by Novikov [222], for *most* potentials in an open dense subset of the Sobolev space $W^{1,\infty}$ by Sun and Uhlmann [261], later by the same authors for *discontinuous* potentials in $L^\infty(\mathbb{V})$ [262], for special kinds of potentials by Nachman [219] (though not necessarily for fixed $\kappa > 0$), and for a broad class of potentials at *almost all* fixed $\kappa \in \mathbb{R}_+$ by Eskin [128]. In some cases [218, 219] the proofs are *constructive* and yield algorithms for inversion. More generic results give practitioners courage to try inversion, but provide little specific guidance as to exactly how much information is really required. Most of the results, with some exceptions that we will explore below, require a continuum of far field measurements from a continuum of incident field directions. Negative results would indeed be useful, though very few are known that indicate when the information is *not* sufficient for unique recovery.

4.4.1 Where Is the Scatterer? How Big Is It?

The first thing we might naturally want to know about the scatterer is where it is and, approximately, how big it is. The first method we study appeared in [205] and belongs to a class of algorithms that share similar features. With these methods one constructs an *indicator function* $\mu : \mathbb{R}^2 \to \mathbb{R} \cup \{\infty\}$ from a test domain Ω_t and the far field pattern u^∞ for a fixed incident direction $-\widehat{x}$. These far field measurements correspond to a segment of a column of the matrix shown in Figure 4.2. The indicator function μ is *small* for all $z \in \mathbb{R}^2$ such that $\Omega \subset \Omega_t + z$, where $\Omega_t + z$ is the shifted test domain, and *infinite* for those z where $\Omega_t + z \cap \Omega = \emptyset$. The size of the test domain Ω_t and the set of points $\{z \in \mathbb{R}^2 \mid \mu(z;\Omega_t,u^\infty(\mathbb{S},-\widehat{x})) < \infty\}$ will determine the approximate size and location of the scatterer. A crucial advantage of this method and others like it [171, 237] is that they only require *one* incident wave (single frequency and single incident direction).

Definition 4.4 (Scattering Test Response). Given the far field pattern $u^\infty(\widehat{\eta}, -\widehat{x})$ for $\widehat{\eta} \in \mathbb{S}$ due to an incident plane wave $u^i(\cdot, -\widehat{x})$ with fixed direction $-\widehat{x}$, let $v_g^i \equiv (\mathscr{H}g)(x)$ denote the incident field defined by (4.18) and $v_g^\infty(\widehat{x})$ denote the corresponding far field pattern given by (4.21). We define the Scattering Test Response for the test domain Ω_t by

$$\mu(z; \Omega_t, u^\infty(\mathbb{S}, -\widehat{x})) \tag{4.33}$$
$$:= \sup\left\{ \left| v_g^\infty(\widehat{x}) \right| \;\middle|\; g \in L^2(\mathbb{S}) \text{ with } \|v_g^i\|_{L^2(\partial(\Omega_t+z))} = 1 \right\}.$$

Theorem 4.5 (Behavior of the Scattering Test Response). *Let the bounded domain Ω_t have a C^2 boundary. If $\Omega \subset \Omega_t + z$, then there is a constant $c \in \mathbb{R}$ such that*

$$\mu(z; \Omega_t, u^\infty(\mathbb{S}, -\widehat{x})) \le c.$$

If, on the other hand, $\overline{\Omega} \cap \overline{\Omega_t + z} = \emptyset$, and $\mathbb{R}^2 \setminus (\overline{\Omega} \cup \overline{(\Omega_t + z)})$ is connected, then we have

$$\mu(z; \Omega_t, u^\infty(\mathbb{S}, -\widehat{x})) = \infty.$$

Proof: A similar version of this theorem was proved in [205, Theorem 3.2]. Without loss of generality, we consider the scattering test response for the unshifted test domain $\mu(0; \Omega_t, u^\infty(\mathbb{S}, -\widehat{x}))$ so that we needn't carry the shift term z throughout the argument.

First, note that the operator $\mathscr{S} : C(\partial\Omega) \to L^2(\mathbb{S})$ that maps the boundary values of radiating solutions to the Helmholtz equation $v^s \in C^2(\Omega^o) \cap C(\overline{\Omega^o})$ to the far field pattern v^∞ can be extended to an injective bounded linear operator $\mathscr{S} : L^2(\partial\Omega) \to L^2(\mathbb{S})$ [98, Theorem 3.21]. Hence, when $\Omega \subset \Omega_t$, for all $v_g^i(x) = \int_{\mathbb{S}} u^i(x, -\widehat{\eta}) g(\widehat{\eta})\, ds(\widehat{\eta})$ satisfying

$$\left\| v_g^i \right\|_{L^2(\partial\Omega_t)} = 1,$$

we have that $v_g^s(x) = \int_{\mathbb{S}} u^s(x, -\widehat{\eta}) g(-\widehat{\eta})\, ds(\widehat{\eta})$ is a radiating solution to the Helmholtz equation on Ω^o and the corresponding far field pattern is bounded in $L^2(\mathbb{S})$. But since the far field $u^\infty(\cdot, -\widehat{x})$ is analytic with respect to $\widehat{x}$, then v_g^∞ is also analytic, and hence pointwise bounded. That is, there is some $c \in \mathbb{R}$ such that

$$|v_g^\infty(\widehat{x})| \le c \quad \text{and hence} \quad \mu(0; \Omega_t, u^\infty(\mathbb{S}, \widehat{x})) \le c$$

for $v_g^\infty(\widehat{x}) = \int_{\mathbb{S}} u^\infty(\widehat{x}, -\widehat{\eta}) g(-\widehat{\eta})\, ds(\widehat{\eta}) = \int_{\mathbb{S}} u^\infty(\widehat{\eta}, -\widehat{x}) g(-\widehat{\eta})\, ds(\widehat{\eta})$ by the reciprocity relation (4.17). This completes the proof of the first statement.

We give the main idea of the proof of the second statement, avoiding technicalities, to which we will point at the end of this discussion. Choose $y \notin \overline{\Omega_t} \cup \overline{\Omega}$ such that the far field pattern $\Phi^\infty(\widehat{x}, y)$ for scattering of an incident point source

$\Phi(\cdot, y)$ by Ω is not zero. This is always possible since, by the *mixed reciprocity relation* [203, Lemma 3.1], we have, for β given by (4.10),

$$\Phi^\infty(\widehat{x}, y) = \beta u^s(y, -\widehat{x}), \tag{4.34}$$

and $u^s(\cdot, -\widehat{x})$ cannot vanish on an open subset of $\mathbb{R}^2$. Next, we use the Herglotz wave operator $\mathscr{H} : L^2(\mathbb{S}) \to L^2(\partial(\Omega_t \cup \Omega))$ to construct an incident field defined by

$$(\mathscr{H} g)(x) := v_g^i(x)\Big|_{\partial(\Omega_t \cup \Omega)},$$

satisfying

$$\left\|v_g^i\right\|_{L^2(\partial\Omega_t)} = 1 \quad \text{and} \quad \left\|v_g^i - \gamma\Phi(\cdot, y)\right\|_{L^2(\partial\Omega)} \leq b(\gamma) \quad (\gamma > 0). \tag{4.35}$$

This is *almost always* possible since the Herglotz wave operator is *almost always* injective with dense range on $L^2(\partial(\Omega_t \cup \Omega))$ [99]. Here $b(\gamma) \in \mathbb{R}$ is chosen so that, by the boundedness of the linear mapping $\mathscr{S} : L^2(\partial\Omega) \to L^2(\mathbb{S})$ of boundary values of radiating solutions to the Helmholtz equation, $w^s \in C^2(\Omega^o) \cap C(\overline{\Omega^o})$ with $w^s = -v_g^i + \gamma\Phi(\cdot, y)$ on Ω, to the far field pattern $w^\infty \equiv v_g^\infty(\widehat{x}) - \gamma\Phi^\infty(\widehat{x}, y)$, we have

$$\left|v_g^\infty(\widehat{x}) - \gamma\Phi^\infty(\widehat{x}, y)\right| \leq c, \tag{4.36}$$

for some fixed constant c and all $\gamma > 0$.

By definition of the scattering test response, we have

$$\mu(0; \Omega_t, u^\infty(\mathbb{S}, -\widehat{x})) \geq \left|v_g^\infty(\widehat{x})\right|, \tag{4.37}$$

and by the triangle inequality applied to (4.36)

$$\left|v_g^\infty(\widehat{x})\right| \geq \gamma|\Phi^\infty(\widehat{x}, y)| - c \tag{4.38}$$

for all $\gamma > 0$. Together, (4.35)–(4.38) yield

$$\mu(0; \Omega_t, u^\infty(\mathbb{S}, -\widehat{x})) \geq \gamma|\Phi^\infty(\widehat{x}, y)| - c$$

for all $\gamma > 0$.

The *almost always* caveat can be removed by choosing a slightly larger domain $\Omega_t' \cap \Omega'$ if necessary. This completes the proof. □

Definition 4.6 (Corona of Ω). Define the corona of the scatterer Ω, relative to the scattering test response μ given in (4.33) and parameterized by the test domain Ω_t and the far field pattern $u^\infty(\cdot, -\widehat{x})$:

$$\mathbb{M}_\mu := \bigcup_{\substack{z \in \mathbb{R}^2 \\ s.t.\ \mu(z; \Omega_t, u^\infty(\mathbb{S}, -\widehat{x})) < \infty}} \Omega_t + z. \tag{4.39}$$

Corollary 4.7 (Approximate Size and Location of Scatterers). *Let* $\Omega_t \subset \mathbb{R}^2$*, with* $\mathbb{R}^2 \setminus \overline{\Omega_t}$ *connected, be a bounded domain large enough that there is some* $z \in \mathbb{R}^2$ *for which* $\Omega \subset \Omega_t + z$*. Then we have*

$$\mathbb{M}_\mu \subset \bigcup_{z \in \mathbb{R}^2} \left\{ \Omega_t + z \,\middle|\, \overline{(\Omega_t + z)} \cap \overline{\Omega} \neq \emptyset \right\} \tag{4.40}$$

and the scatterer Ω *is a subset of its corona,* $\mathbb{M}_\mu$*.*

Proof: For points z with $\mu(z;\Omega_t, u^\infty(\mathbb{S}, -\widehat{x})) < \infty$, by Theorem 4.5 we have $\overline{(\Omega_t + z)} \cap \overline{\Omega} \neq \emptyset$, from which we immediately obtain the relation (4.40). For $\Omega \subset \Omega_t + z$ we have $\mu(z;\Omega_t, u^\infty(\mathbb{S}, -\widehat{x})) < \infty$, and thus the support of the scatterer is a subset of its corona. □

Before we develop the numerical algorithm based on these facts, we would like to point out some challenges in the theory above. The observant reader will notice that we didn't mention what happens to μ when $\Omega \cap (\Omega_t + z) \neq \emptyset$ but $\Omega \cap (\mathbb{R}^2 \setminus (\Omega_t + z)) \neq \emptyset$. If $\mu(z;\Omega_t, u^\infty(\mathbb{S}, -\widehat{x})) = \infty$ when $\Omega \cap (\Omega_t + z) \neq \emptyset$ but $\Omega \cap (\mathbb{R}^2 \setminus (\Omega_t + z)) \neq \emptyset$, then the set inequality (4.40) can be tightened considerably. Unfortunately, because the fields can be analytically continued, the answer to this question is not as sharp as we might hope. Also note that the constant c in Theorem 4.5 is not resolved. All we know is that c is smaller than infinity, but that isn't saying much. Naturally, we would like to know more about this constant. Finally, note that the optimization problem embedded in (4.33) is an infinite-dimensional problem which we must solve at *each* point $z \in \mathbb{D}$, now interpreted as some computational domain similar to the experimental domain used in Section 4.2. Even with all these challenges, we can get a surprising amount of information from a naive implementation of this test, as we demonstrate below.

We address first the computation of the scattering test response μ. By (4.33), we must solve, at each point z, an optimization problem over the densities $g \in L^2(\mathbb{S})$. It is not possible to search over the entire infinite-dimensional space. Instead, we search over a well-chosen sample of this space. That is, we search over the densities such that the incident field $v^i_{g_*}$ approximates the fundamental solution $\Phi(x,y)$ on $x \in \partial(\Omega_t + z)$ for $y \in \mathbb{R}^2 \setminus \overline{(\Omega_t + z)}$. At each point $z \in \mathbb{D}$ we solve the following ill-posed equation for g_*:

$$v^i_{g_*}(x) = \Phi(x,y) \text{ for } x \in \partial(\Omega_t + z),\; y \in \mathbb{R}^2 \setminus \overline{(\Omega_t + z)}, \tag{4.41}$$

where $v^i_{g_*}$ is given by (4.18). Of course, $\|v^i_{g_*}\| \neq 1$, but we can fix this by scaling the density g_*.

Denote the Herglotz wave operator corresponding to this superposition of plane waves $v^i_{g_*}$ by $\mathscr{H}_z$. Since (4.41) is ill-posed, we solve the Tikhonov-regularized least-squares problem

$$\underset{g\in L^2(\mathbb{S})}{\text{minimize}} \ \|\mathscr{H}_z g - \Phi(\cdot,y)\|^2_{L^2(\partial(\Omega_t+z))} + \alpha\|g\|^2 \tag{4.42}$$

whose solution is

$$g_*(\cdot;y,z,\alpha) := (\alpha I + \mathscr{H}_z^*\mathscr{H}_z)^{-1}\mathscr{H}_z^*\Phi(\cdot,y). \tag{4.43}$$

This yields

$$v^i_{g_*}(\cdot;y,z,\alpha) \ \approx \ \Phi(\cdot,y) \quad \text{on } \partial(\Omega_t+z).$$

We thus exchange the infinite-dimensional optimization problem in (4.33) for the parameterized, finite-dimensional optimization problem

$$\mu(z;\Omega_t,u^\infty(\mathbb{S},-\widehat{x})) = \sup_{y\in\mathbb{R}^2}\left|v_g^\infty(\widehat{x};y,z,\alpha)\right|, \tag{4.44}$$

where g is the normalized density

$$g = \frac{g_*}{\|v^i_{g_*}\|} \qquad \Longrightarrow \qquad \|v^i_g\| = 1.$$

Next, we introduce a specific approximation domain that allows further efficiencies due to symmetry of the fundamental solution Φ. Let our test domain Ω_t be a circle of radius t centered on the origin. In [202, Proposition 2] it is shown that

$$g(\widehat{\eta};y,z,\alpha) = e^{-i\kappa z\cdot\widehat{\eta}}g(\widehat{\eta};y,0,\alpha), \tag{4.45}$$

where g is the solution to (4.42). Similarly, rotations of the point y around the origin translate to shifts in the density with respect to $\mathbb{S}$:

$$g(\widehat{\eta};R_{\widehat{w}}y,z,\alpha) = e^{-i\kappa z\cdot\widehat{\eta}}g(R_{-\widehat{w}}\widehat{\eta};y,0,\alpha), \tag{4.46}$$

where $R_{\widehat{w}}$ is the rotation by $\widehat{w}$ in the plane. Thus, for fixed $t>0$ with $y = R_{\widehat{w}}t\widehat{y}_0$, where $\widehat{y}_0 \in \mathbb{S}$ is a reference direction, we have the explicit, closed-form expressions for the densities g:

$$g(\widehat{\eta};y,z,\alpha) = e^{-i\kappa z\cdot\widehat{\eta}}g(R_{-\widehat{w}}\widehat{\eta};t\widehat{y}_0,0,\alpha), \tag{4.47}$$

where

$$g(\widehat{\eta};t\widehat{y}_0,0,\alpha) = \left((\alpha I + \mathscr{H}_0^*\mathscr{H}_0)^{-1}\mathscr{H}_0^*\Phi\right)(\widehat{\eta};t\widehat{y}_0), \tag{4.48}$$

and $\mathscr{H}_0$ is the Herglotz wave operator restricted to the test domain centered on the origin, $\Omega_t + 0$. We need only compute (4.48) along the line $t>0$ and solve (4.44) for these explicitly calculated densities.

In the absence of a satisfactory algorithm for the solution of (4.44), we propose the following technique whose justification we shall not pursue here.

Algorithm 4.8 (Partial Scattering Response).

Step 0: Choose $\varepsilon > 0$ and Ω_t, a circle of radius t centered at the origin where t is large enough that $\Omega \subset \Omega_t + z$ for some $z \in \mathbb{R}^2$.

Step 1: Let $g(\widehat{\eta}, (t+\varepsilon)\widehat{y}, z, \alpha)$ be given by (4.47) with

$$g(\widehat{\eta}, (t+\varepsilon)\widehat{y}_0, 0, \alpha) = \left((\alpha I + \mathscr{H}_0^* \mathscr{H}_0)^{-1} \mathscr{H}_0^* \Phi\right)(\widehat{\eta}, (t+\varepsilon)\widehat{y}_0) \quad (4.49)$$

for the fundamental solution $\Phi(x, (t+\varepsilon)\widehat{y}_0)$ with source point located at $(t+\varepsilon)\widehat{y}_0$.

Step 2: For an arbitrary, fixed $\widehat{x} \in \mathbb{S}$, at each sample point $z \in \mathbb{D}$, the computational domain, compute the *partial scattering test response*, $\delta : \mathbb{R}^2 \to \mathbb{R}_+$, defined by

$$\delta(z, \widehat{x}) \equiv \int_{\mathbb{S}} |(\mathscr{F} g(\widehat{\eta}, (t+\varepsilon)\widehat{y}, z, \alpha))(\widehat{x})| \; ds(\widehat{y}) \quad (4.50)$$

where and $\mathscr{F}$ is the far field operator defined by (4.23).

Step 3: Plot the graph of $\delta(z, \widehat{x})$ at each sample point z.

For the above algorithm to yield a useful image, the following must hold:

Proposition 4.9 (Discontinuity in the Partial Scattering Test Response). *For any $\widehat{x} \in \mathbb{S}$, there exist constants $0 < M' < M$ such that*

$$\delta(z) \begin{cases} > M & \forall\, z \in \mathbb{R}^2 \quad \text{where} \quad \Omega \cap \Omega_t + z = \varnothing; \\ < M' & \forall\, z \in \mathbb{R}^2 \quad \text{where} \quad \Omega \subset \Omega_t + z. \end{cases} \quad (4.51)$$

Using the efficient formulation (4.47), we need only solve one ill-posed integral equation, (4.49), and calculate the integral in (4.50) at each sample point z. The corona of the scatterer is identified by a jump in $\delta(z)$. Rather than proving the above proposition, we test its plausibility numerically.

If Proposition 4.8 is true, then the scatterer lies in the domain $\mathbb{G} + \Omega_t$ where Ω_t is a circle centered on the origin and $\mathbb{G}$ is the set of points $z \in \mathbb{D}$ where (4.51) is satisfied. To generate Figure 4.3 we used a test domain radius of $t = 5\sqrt{2}$. In order to cover the domain $\mathbb{D} = [-100, 100] \times [-100, 100]$, this required us to sample on a 20×20 grid for a pixel size of 10×10. The dark region $\mathbb{G}$ shown in the figure are the points z on this grid where (4.51) is satisfied with $M = 9$, indicating that there is something of interest in the region $\mathbb{G} + \Omega_t$.

There are two principal advantages of this method: First, only a single incident direction $\widehat{x}$ is needed, and, second, one can cast as large a net as desired, depending on the radius of the test domain Ω_t, in order to determine the approximate location and size of the scatterer without the need to sample at many points $z \in \mathbb{D}$. We will see in Section 4.4.3 whether the conjectured region does indeed contain something of interest.

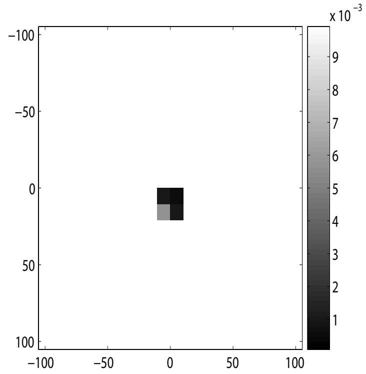


Figure 4.3. Plotted is the value of the integral in (4.51) at the reference points $z \in \mathbb{D}$, where $\mathbb{D}$ is shown in Figure 4.1(a). The test domain Ω_t is a circle of radius $t = 5\sqrt{2}$ and with a cutoff value in (4.51) of $M = 9$. If Proposition 4.8 is true, then the scatterer lies in the region $\mathbb{G} + \Omega_t$, where $\mathbb{G}$ is the set of points in the dark region above.

4.4.2 Is the Scatterer Absorbing?

Recall from Section 4.3 that the scattered field we seek lies in the range of the far field operator $\mathscr{F}$ defined by (4.23). The first question that comes to mind, then, regarding the range of $\mathscr{F}$ is, what are its spectral properties, that is, how do its eigenvalues behave. We obtain a partial answer with the next theorem.

Theorem 4.10. [246] *The far field operator has at most a countable number of discrete eigenvalues with zero as the only cluster point.*

Proof: This follows from the fact that $\mathscr{F}$ is a compact operator [249]. □

This is disappointing. Even if zero is not an eigenvalue, the decay of the eigenvalues of $\mathscr{F}$ will cause numerical instabilities and sensitivity to noise in the determination of the range of $\mathscr{F}$. This is symptomatic of *ill-posed problems* like the one we are faced with here. While the spectral properties of the far field operator point to some of the difficulties in recovering scatterers from far field measurements, the next theorem, due to Colton and Kress [97], shows that the spectrum of $\mathscr{F}$ easily provides qualitative information about the nature of the scatterer, whether it is absorbing or not, from the location of the eigenvalues of $\mathscr{F}$.

Theorem 4.11. *Let the scattering inhomogeneity have index of refraction defined in (4.4) mapping $\mathbb{R}^2$ to the upper half of the complex plane. The scattering inhomogeneity is nonabsorbing, that is, $\Im n(x) = 0$ for all x, if and only if the eigenval-*

ues of $\mathscr{F}$ lie on the circle centered at $\frac{1}{2\kappa}\left(\Im(\beta^{-1}),\Re(\beta^{-1})\right)$ and passing through the origin. Otherwise, the eigenvalues of $\mathscr{F}$ lie on the interior of this disk.

Proof: This is a restatement of [98, Corollary 8.19], the proof of which we collect here for ease of reference. Interested readers are also referred to [97]. Let $v_g = v_g^i + v_g^s$ satisfy (4.3) with v_g^s satisfying (4.8) and v_g^i defined by (4.18) where $g \in L^2(\mathbb{S})$ is an eigenfunction of $\mathscr{F}$, that is, $\mathscr{F}g = \lambda g$. By (4.12) we have

$$\int_\Omega (\overline{v_g}\Delta v_g - v_g\Delta\overline{v_g})\,dx = \int_{\partial\Omega} \overline{v_g}\frac{\partial v_g}{\partial\nu} - v_g\frac{\partial\overline{v_g}}{\partial\nu}\,ds. \tag{4.52}$$

But v_g satisfies (4.3) so the left-hand side of (4.52) satisfies

$$\int_\Omega (\overline{v_g}\Delta v_g - v_g\Delta\overline{v_g})\,dx = -2\kappa^2 i\int_\Omega \Im(n(x))|v_g(x)|^2\,dx. \tag{4.53}$$

According to (4.2), the right-hand side of (4.52) can be expanded to

$$\begin{aligned}\int_{\partial\Omega} \overline{v_g}\frac{\partial v_g}{\partial\nu} - v_g\frac{\partial\overline{v_g}}{\partial\nu}\,ds &= \int_{\partial\Omega} \overline{v_g^s}\frac{\partial v_g^s}{\partial\nu} - v_g^s\frac{\partial\overline{v_g^s}}{\partial\nu}\,ds\\ &\quad - 2i\Im\int_{\partial\Omega} \overline{v_g^s}\frac{\partial v_g^i}{\partial\nu} - v_g^i\frac{\partial\overline{v_g^s}}{\partial\nu}\,ds\\ &\quad + \int_{\partial\Omega} \overline{v_g^i}\frac{\partial v_g^i}{\partial\nu} - v_g^i\frac{\partial\overline{v_g^i}}{\partial\nu}\,ds\\ &= \int_{\partial\Omega} \overline{v_g^s}\frac{\partial v_g^s}{\partial\nu} - v_g^s\frac{\partial\overline{v_g^s}}{\partial\nu}\,ds\\ &\quad - 2i\Im\int_{\partial\Omega} \overline{v_g^s}\frac{\partial v_g^i}{\partial\nu} - v_g^i\frac{\partial\overline{v_g^s}}{\partial\nu}\,ds.\end{aligned} \tag{4.54}$$

Now, (4.8) gives

$$v_g^s\frac{\partial\overline{v_g^s}}{\partial\nu} = \frac{-i\kappa}{|x|}v_g^\infty\overline{v_g^\infty} + O\left(\frac{1}{|x|^2}\right), \qquad |x|\to\infty.$$

So by (4.13),

$$\int_{\partial\Omega} \overline{v_g^s}\frac{\partial v_g^s}{\partial\nu} - v_g^s\frac{\partial\overline{v_g^s}}{\partial\nu}\,ds = 2i\kappa\int_{\mathbb{S}} |v_g^\infty|^2\,ds. \tag{4.55}$$

Expanding the expression for v_g^i, together with a change in the order of integration and (4.16) yields

$$\begin{aligned}\int_{\partial\Omega} \overline{v_g^s}\frac{\partial v_g^i}{\partial\nu} - v_g^i\frac{\partial\overline{v_g^s}}{\partial\nu}\,ds &= \int_{\mathbb{S}} g(\widehat{y})\int_{\partial\Omega} \overline{v_g^s}\frac{\partial e^{i\kappa\widehat{y}\cdot x}}{\partial\nu} - e^{i\kappa\widehat{y}\cdot x}\frac{\partial\overline{v_g^s}}{\partial\nu}\,ds(x)\,ds(\widehat{y})\\ &= \overline{\beta^{-1}}\int_{\mathbb{S}} g(\widehat{y})\overline{v_g^\infty}(\widehat{y})\,ds(\widehat{y}).\end{aligned} \tag{4.56}$$

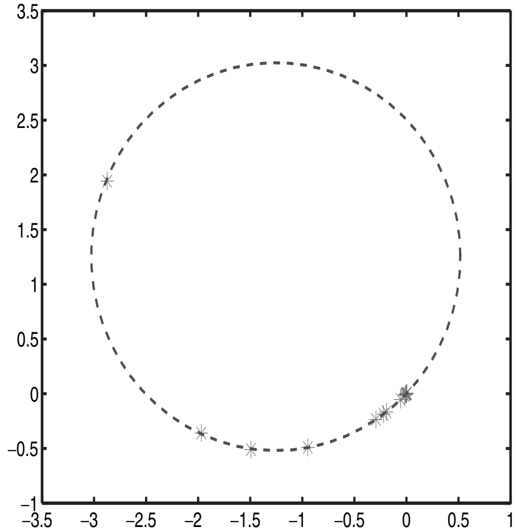


Figure 4.4. The eigenvalues (asterisks) of the far field matrix shown in Figure 4.2 are shown to line up on the circle passing through the origin with center $1/2\kappa(\Im\beta, \Re\beta)$ for $\kappa = 2$ and β given by (4.10). This implies that the inhomogeneity is nonabsorbing.

In summary, (4.52)–(4.56) give

$$\begin{aligned} -2\kappa^2 i \int_\Omega \Im(n(x))|v_g(x)|^2\, dx &= 2i\kappa \int_{\mathbb{S}} |v_g^\infty|^2\, ds + \overline{\beta^{-1}} \int_{\mathbb{S}} g(\widehat{y})\overline{v_g^\infty}(\widehat{y})\, ds(\widehat{y}) \\ &\quad -\beta^{-1} \int_{\mathbb{S}} \overline{g}(\widehat{y}) v_g^\infty(\widehat{y})\, ds(\widehat{y}) \\ &= 2i\kappa \int_{\mathbb{S}} |v_g^\infty|^2\, ds - 2i\Im\left(\beta^{-1}\left\langle v_g^\infty, g\right\rangle\right). \end{aligned}$$

By (4.20) we have that $\mathscr{F}g = v_g^\infty$, and since g is an eigenfunction of $\mathscr{F}$, we have

$$-\frac{\kappa}{||g||^2} \int_\Omega \Im(n(x))|v_g(x)|^2\, dx = |\lambda|^2 - \Im\left(\frac{\lambda}{\kappa\beta}\right). \tag{4.57}$$

This completes the proof. □

As Figure 4.4 shows, the eigenvalues of the sampled far field operator corresponding to our data set lie on the circle passing through the origin with center

$$1/2\kappa(\Im\beta, \Re\beta) = \sqrt{\pi}\left(-\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2}\right)$$

for $\kappa = 2$ and β given by (4.10). From the previous theorem we conclude that the scatterer is nonabsorbing.

In some applications, this may be all that is needed to distinguish whether the scatterer is of interest. For instance, the presence of leukemia causes the bone marrow to exhibit an elevated electric permittivity and diminished conductivity as compared to a healthy individual. This difference can, in theory, be detected by a shift in the location of the eigenvalues of the far field operator corresponding to electromagnetic measurements analogous to the data shown in Figure 4.2 [102]. Whether this is a viable diagnostic tool depends on a number of factors: the sensitivity of the eigenvalues to electrical parameter shifts; whether the shift, or *signal* can be distinguished from random variations, or *noise*; and whether the amount of data needed to achieve a sufficient signal is practical—i.e., the required electromagnetic radiation should not do more damage to the patient than the disease!

4.4.3 What Is the Shape of the Scatterer?

We now use the information from the previous method to refine our search of the domain $\mathbb{D}$ with the goal of determining the approximate shape of the scatterer. The method we shall explore is the *linear sampling* method developed by Colton, Kirsch, and others [96,104,7,215,95]. As with the method in the previous section, this method and others like it [236,179,100,101] use the blow-up of some function to indicate whether a sampled point $z \in \mathbb{R}^2$ is on the interior of the unknown scatterer. The linear sampling method is a type of *feasibility* test for the solution of what is known as the *interior transmission problem.* This partial differential equation is recast as a linear integral equation parameterized by z where the kernel of integral operator is the far field data u^∞. This corresponds to the interpretation of the data as forming the operator defined by (4.23) whose spectral properties tell us about the boundary values of the partial differential equation that generated this kernel. This is in contrast to the view of *backpropagation* represented by (4.24) whereby we seek to reverse the scattering process back to the source. It is shown that the interior transmission problem almost always has at most one solution, and if $z \in \Omega$ then a solution does indeed exist. Moreover, as $z \to \partial\Omega$ from the interior of Ω, then the solution to the related linear integral equation becomes unbounded, indicating the infeasibility of the interior transmission problem. We use the blow-up of this putative solution to image the boundary of the scatterer. This is described in more detail next.

To begin, we define the interior transmission problem:

$$\triangle w(x) + \kappa^2 n(x) w(x) = 0, \quad \triangle v(x) + \kappa^2 v(x) = 0 \text{ for } x \in \Omega, \tag{4.58}$$

$$w - v = f(\cdot, z), \quad \frac{\partial w}{\partial \nu} - \frac{\partial v}{\partial \nu} = \frac{\partial f}{\partial \nu} \quad \text{on } \partial\Omega. \tag{4.59}$$

From our first experiment, shown in Figure 4.4, we have determined that the medium that generated the data shown in Figure 4.2 is nonabsorbing, that is, $\Im(n(x)) = 0$ for all x. If it had been even slightly absorbing ($\Im(n(x)) > 0$ as would most likely be the case for any physical data), then we could have been certain that there are no nontrivial solutions to the homogeneous problem (4.58)–(4.59) with $f = 0$, hence the inhomogeneous problem will have a unique solution when a solution exists. But even in our case, it was shown [103] that the set of values of κ for which the solution to (4.58)–(4.59) with $f = 0$ has a nontrivial solution—called *transmission eigenvalues*—is a discrete set. We can therefore be almost sure that, for our data, κ is *not* a transmission eigenvalue.

We observe further the following fact.

Theorem 4.12. [98, Theorem 8.10] *Let*

$$f(y) = h_p^{(1)}(\kappa|y|)Y_p(\widehat{y}), \tag{4.60}$$

a spherical wave function of order p, and let β be given by (4.10). The integral equation

$$\int_{\mathbb{S}} u^\infty(\widehat{x};\widehat{y})g(-\widehat{x})\, ds(\widehat{x}) = \frac{i^{p-1}}{\beta\kappa} Y_p(\widehat{y}), \qquad \widehat{y} \in \mathbb{S}, \tag{4.61}$$

has a solution $g \in L^2(\mathbb{S})$ if and only if there exists $w \in C^2(\Omega) \cap C^1(\overline{\Omega})$ and a function v given by

$$v(x) = \int_{\mathbb{S}} e^{i\kappa x\cdot(-\widehat{y})} g(-\widehat{y})\, ds(\widehat{y}) \tag{4.62}$$

such that the pair (w, v) is a solution to (4.58)–(4.59).

Proof: Let $w^i \equiv v$ and $w^s \equiv f$. Then w solves the scattering problem

$$\left(\triangle + \kappa^2 n(x)\right) w(x) = 0 \text{ for } x \in \mathbb{R}^2, \tag{4.63}$$

$$w = f + v, \tag{4.64}$$

$$r^{\frac{1}{2}}\left(\frac{\partial}{\partial r} - i\kappa\right) f(x) \to 0, \;\; r = |x| \to \infty. \tag{4.65}$$

The solution to this problem is also the solution to the interior transmission problem (4.58)–(4.59). (Note that v given by (4.62) is an entire solution to the Helmholtz equation.) Now, by (4.20) and the observation that

$$f(y) = \frac{e^{i\kappa|y|}}{|y|^{1/2}} \frac{i^{p-1}}{\kappa} Y_p(\widehat{y}) + o\left(\frac{1}{|y|^{1/2}}\right), \qquad \widehat{y} = \frac{y}{|y|},$$

we have that $w^\infty(\widehat{y}) = \frac{i^{p-1}}{\beta\kappa} Y_p(\widehat{y})$. Hence, the solvability of (4.58)–(4.59) is equivalent to the solvability of (4.61). □

Finally, it can be shown [98, Theorem 10.25] that there exists a unique weak solution to (4.58)–(4.59) with $f(x;z) \equiv \Phi(x,z)$ for every $z \in \Omega$ with Φ given by (4.15), that is, the pair (w,v) satisfies

$$(I + \kappa^2 \mathscr{V})w = v \qquad \text{on } \Omega \tag{4.66}$$

and

$$-\kappa^2 \mathscr{V} w = \Phi(\cdot, z) \qquad \text{on } \partial\mathbb{B}, \tag{4.67}$$

where $\mathscr{V}$ is the volume integral defined by (4.25) and $\mathbb{B} \subset \mathbb{R}^2$ is a ball with $\Omega \subset \mathbb{B}$.

To recap the logic thus far, we observe that (4.61) has a solution if and only if there is a corresponding solution to (4.58)–(4.59) with f given by (4.60); moreover, (4.58)–(4.59) with $f = \Phi(x,z)$ is solvable for every $z \in \Omega$. The natural thing to ask is, for $z \in \mathbb{R}^2 \setminus \Omega$, or, just as $z \to \partial\Omega$ from inside Ω, what happens to solutions to

$$\int_{\mathbb{S}} u^\infty(\widehat{x};\widehat{y}) g(-\widehat{x})\, ds(\widehat{x}) = \Phi^\infty(\widehat{y}, z), \qquad \widehat{y} \in \mathbb{S}, \tag{4.68}$$

where $\Phi^\infty(\widehat{y}, z)$ is the far field pattern of the fundamental solution $\Phi(y,z)$?

Theorem 4.13 (Linear Sampling). *For every $\varepsilon > 0$ and $z \in \Omega$ there exists a $g(\cdot;z) \in L^2(\mathbb{S})$ satisfying*

$$\|\mathscr{F} g - \Phi^\infty(\cdot, z)\|_{L^2(\mathbb{S})} \le \varepsilon \tag{4.69}$$

such that

$$\lim_{z\to\partial\Omega} \|g\|_{L^2(\mathbb{S})} = \infty \quad \textit{and} \quad \lim_{z\to\partial\Omega} \|v_g\|_{L^2(\Omega)} = \infty, \tag{4.70}$$

where v_g is given by (4.18). If instead $z \in \Omega^o$, then for every $\varepsilon, \delta > 0$ there is a $g(\cdot;z) \in L^2(\mathbb{S})$ satisfying

$$\|\mathscr{F} g - \Phi^\infty(\cdot, z)\|_{L^2(\mathbb{S})} \le \varepsilon + \delta \tag{4.71}$$

such that

$$\lim_{\delta\to 0} \|g\|_{L^2(\mathbb{S})} = \infty \quad \textit{and} \quad \lim_{\delta\to 0} \|v_g\|_{L^2(\Omega)} = \infty, \tag{4.72}$$

where v_g is given by (4.18).

Proof: This result has developed since 1996. Pieces of it can be found in [96, 104, 79, 95]. The latter two of these references contain the current extent of the theory sketched here. Let the pair $(w(\cdot;z), v(\cdot;z))$ be the weak solution to (4.58)–(4.59) with $f = \Phi(\cdot, z)$, that is, w and v satisfy (4.66)–(4.67). Denote the linear space of Herglotz wave functions by

$$\mathbb{H} \equiv \left\{ h \,\middle|\, h(x) = \int_{\mathbb{S}} e^{i\kappa x\cdot\widehat{\eta}} g(\widehat{\eta})\, ds(\widehat{\eta}) \text{ for } g \in L^2(\mathbb{S}) \right\}.$$

For this space, $v \in \overline{\mathbb{H}}$, thus for every $\widetilde{\varepsilon} > 0$ and $z \in \Omega$ there is a $g(\cdot;z) \in L^2(\mathbb{S})$ such that

$$\left\| v(\cdot, z) - v_g(\cdot) \right\|_{L^2(\Omega)} \le \widetilde{\varepsilon}, \tag{4.73}$$

where

$$v_g(x) = \int_{\mathbb{S}} e^{i\kappa x\cdot\widehat{\eta}} g(\widehat{\eta}; z)\, ds(\widehat{\eta}).$$

Next, note that the inverse operator $(I + \kappa^2 \mathscr{V})^{-1}$ is defined and continuous. Thus, for some $c > 0$ and

$$w_g \equiv (I + \kappa^2 \mathscr{V})^{-1} v_g,$$

we have

$$\left\| w(\cdot, z) - w_g(\cdot) \right\|_{L^2(\Omega)} \le c\widetilde{\varepsilon}. \tag{4.74}$$

By the continuity of $\mathscr{V}$, (4.74) yields the following bound:

$$\left\| \kappa^2 \mathscr{V} w_g - \Phi(\cdot, z) \right\|_{C(\partial\mathbb{B})} \le c'\widetilde{\varepsilon}, \tag{4.75}$$

for some $c' > 0$. Denote the scattered field due to the incident field $u^i = e^{i\kappa^2(-\widehat{\eta})}$ by $u^s(x, -\widehat{\eta})$. From (4.19) we have $w_g = v_g - \kappa^2 \mathscr{V} w_g$ and

$$-\kappa^2 \mathscr{V} w_g = \int_{\mathbb{S}} u^s(x, -\widehat{\eta}) g(-\widehat{\eta})\, ds(\widehat{\eta}),$$

hence

$$w_g^\infty(\widehat{x}) \equiv \int_{\mathbb{S}} u^\infty(\widehat{x}, -\widehat{\eta}) g(-\widehat{\eta})\, ds(\widehat{\eta}) = (\mathscr{F} g)(\widehat{x}), \quad \widehat{x} \in \mathbb{S}. \tag{4.76}$$

Note that the solution to the scattering problem on the exterior domain $\mathbb{R}^2 \setminus \mathbb{B}$ depends continuously on the boundary conditions on $\partial\mathbb{B}$, thus

$$\|\mathscr{F} g - \Phi^\infty(\cdot, z)\|_{L^2(\mathbb{S})} \le c''\widetilde{\varepsilon} \tag{4.77}$$

for some $c'' > 0$. Letting $\varepsilon = c''\widetilde{\varepsilon}$ completes the first part of the proof.

The proof of (4.70) is technical. We sketch the basic idea here and refer the reader to [79, 95] for details. The idea is to use the continuous embedding of $C(\partial\Omega)$ in the Sobolev space $H^{3/2}(\partial\Omega)$ to achieve the bound

$$\|\Phi(\cdot, z)\|_{C(\partial\Omega)} \le c \|\kappa^2 \mathscr{V} w(\cdot, z)\|_{H^{3/2}(\partial\Omega)}.$$

By the Trace theorem and the fact that $(I+\kappa^2\mathscr{V})^{-1}$ and $\mathscr{V}$ are bounded, one obtains the bound

$$\|\kappa^2\mathscr{V}w(\cdot,z)\|_{H^{3/2}(\partial\Omega)} \le c\|v(\cdot,z)\|_{L^2(\Omega)}.$$

Now, combining (4.73) with the previous inequalities yields

$$\|\Phi(\cdot,z)\|_{C(\partial\Omega)} \le c\left(\|v_g\|_{L^2(\Omega)} + \widetilde{\varepsilon}\right),$$

whence the right limit of (4.70). Since v_g with g bounded in $L^2(\mathbb{S})$ is also bounded in $L^2(\Omega)$, the left inequality of (4.70) follows immediately.

To prove (4.72) one analyzes the range of the *far field mapping* $\mathscr{T} : L^2(\Omega) \to L^2(\mathbb{S})$, mapping the total field (scattered plus incident) to the corresponding far field pattern. An important property is that $\Phi^\infty(\cdot,z)$ is in the range of $\mathscr{T}(I-\kappa^2\mathscr{V})^{-1}$, that is, in the range of the far field mapping of solutions to the Lippmann-Schwinger equation (4.29), if and only if $z\in\Omega$. Nevertheless, the operator $\mathscr{T}(I-\kappa^2\mathscr{V})^{-1}$ has dense range on $L^2(\mathbb{S})$ [79], and thus there is $\widetilde{v}$ such that

$$\left\|\mathscr{T}(I-\kappa^2\mathscr{V})^{-1}\widetilde{v} - \Phi^\infty(\cdot,z)\right\|_{L^2(\mathbb{S})} < \delta$$

for any $\delta > 0$. Such a $\widetilde{v}$, in turn, can be approximated arbitrarily closely by a Herglotz wave function v_g, that is, for every $\varepsilon > 0$ there is a g such that

$$\|\widetilde{v} - v_g\|_{L^2(\Omega)} < \varepsilon.$$

The rest then follows from the continuity of $\mathscr{T}(I-\kappa^2\mathscr{V})^{-1}$ and the triangle inequality. For details we refer the reader to [95]. □

The algorithm suggested by Theorem 4.13 follows almost immediately and shares many features of the scattering test response of Section 4.4.1. First note that the equation

$$\mathscr{F}g = \Phi^\infty(\cdot,z) \tag{4.78}$$

is ill-posed, albeit linear, with respect to g. As in Section 4.4.1, we regularize the problem by solving the regularized least squares problem

$$\underset{g\in L^2(\mathbb{S})}{\text{minimize}}\ \|\mathscr{F}g - \Phi^\infty(\cdot,z)\|^2 + \alpha\|g\|^2. \tag{4.79}$$

The solution to this problem is

$$g(\cdot;z,\alpha) \equiv (\alpha I + \mathscr{F}^*\mathscr{F})^{-1}\mathscr{F}^*\Phi^\infty(\cdot,z). \tag{4.80}$$

Since we already know from the scattering test response approximately where and how big the scatterer is, we needn't calculate (4.80) at all points $z\in\mathbb{D}$, but

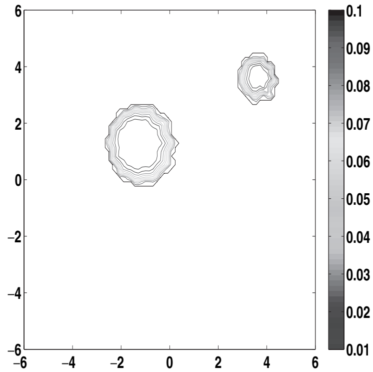


Figure 4.5. Scatterer estimated using the linear sampling method. Shown is $\|g(\cdot;z_j,\alpha)\|_{L^2(\mathbb{S})}$ for $g(\cdot;z_j,\alpha)$ given by (4.80) with $\alpha = 10^{-8}$ for all grid points z_j on the domain $[-6,6]\times[-6,6]$ sampled at a rate of 40 points in each direction.

rather just on the corona $\mathbb{M}_\mu$, or, if Proposition 4.8 holds, then on the corona $\mathbb{M}_\delta$ calculated using δ in (4.50). We identify the boundary of the scatterer by those points z_j on a grid where the norm of the density $g(\cdot;z_j,\alpha)$ becomes large relative to the norm of the density at neighboring points.

In Figure 4.5 we show the value of the level curves of $\|g(\cdot;z_j,\alpha)\|_{L^2(\mathbb{S})}$ at points $z_j \in \mathbb{G} \subset \mathbb{M}_\delta$ with $\alpha = 10^{-8}$. The resulting image indicates that the scatterer consists of two distinct scatterers of different size.

For our implementations we do not take as much care with the choice of the regularization parameter α as we could. A more precise implementation would calculate an optimal α at each sample point z_j [104]. Obviously, since (4.78) is regularized, $\|g(\cdot;z,\alpha)\|_{L^2(\mathbb{S})}$ will be bounded, so a reasonable cutoff will have to be chosen that will affect the estimate for the shape and extent of the boundary of the scatterer. This is clearly a weakness of the technique, but it does not appear in practice to be significant. The contours of Figure 4.5 indicate that the shape estimate is robust with respect to this cutoff.

What is more problematic about linear sampling, however, is that it only says that *there exists* a g that is unbounded in norm. It doesn't tell us how to calculate that g or even how common these densities are. We cannot exclude the possibility of a phantom scatterer consisting of points $z \in \mathbb{R}^2 \setminus \Omega$ satisfying

$$\|\mathscr{F}g - \Phi^\infty(\cdot,z)\|_{L^2(\mathbb{S})} \le \varepsilon \tag{4.81}$$

such that $\|g\|_{L^2(\mathbb{S})}$ is small. We observe, however, that $\|g\|_{L^2(\mathbb{S})}$ remains relatively large for all $z \in \mathbb{R}^2 \setminus \Omega$.

Kirsch [179, 180] amended the linear sampling method to close this gap. In particular, he showed that

$$(\mathscr{F}^*\mathscr{F})^{\frac{1}{4}} g = \Phi^\infty(\cdot, z) \tag{4.82}$$

has a solution if *and only if* $z \in \Omega$. Imaging using $(\mathscr{F}^*\mathscr{F})^{\frac{1}{4}}$ has become known as the *factorization method*. Arens [7] later showed that in certain cases the density computed by (4.80) corresponds to a Tikhonov-regularized solution to (4.82), thus, in this setting, the linear sampling is indistinguishable from the more rigorous method of Kirsch. This is indeed a remarkable coincidence since it is not at all obvious why one would use Tikhonov regularization (or others like it, including More-Penrose inversion) other than the fact that it is easy to implement. Had a different regularization, such as maximum entropy, been the method of choice, linear sampling might not have worked so well, and Kirsch's analysis might never have been pursued!

Remark 4.14 (Open Problem). Does there exist a regularization of (4.78) such that the linear sampling method is guaranteed to fail?

Current research on the limited sampling algorithm, Kirsch's factorization method, and similar approaches involves applying the techniques in ever more complicated settings. The numerical tests of feasibility for these techniques are often easy to set up and become easier as one's test case software becomes more sophisticated. Given the accessibility of software tools, it is very natural that the research would proceed by first doing a numerical test, and then doing the theoretical work to explain the results of the test. This is a central feature of modern experimental mathematics.

4.4.4 Refining the Information

To maintain some sense of mystery about the scatterer that we are trying to tease out of the data in Figure 4.2, we have purposely withheld the true answer to each of the above queries about the nature of the scatterer. Unfortunately, inverse scattering is not like an Arthur Conan Doyle novel—there is never a tipping point in our investigation in which, with all the clues in place, we can simply deduce the solution. We still need to peek at the answer to see if we are on the right track. To close this case study, we reveal the true answer in order to see how we did, and we discuss current trends for refining the information. The true scatterer was a series of six circles, two with radius 0.5 centered at $(0,0)$ and $(3,3)$ and four with radius 1 centered at $(\pm 1, \pm 1)$. The circles centered at $(0,0)$, $(-1,-1)$, $(1,1)$, and $(1,-1)$ all had an index of refraction of $n(x) = \frac{401}{400}$, while the circles centered at $(3,3)$ and $(-1,1)$ had $n(x) = 201$ and $n(x) = 401$, respectively.

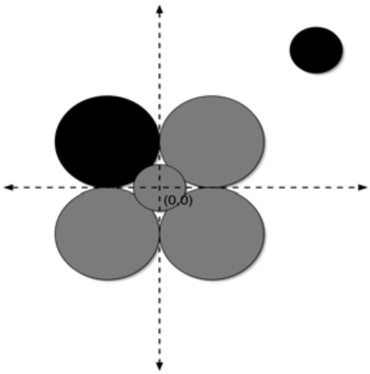


Figure 4.6. The true scatterer consisting of six circles of different sizes and indices of refraction indicated by grayscale.

We correctly located the scatterer and determined its approximate size using the partial scattering test response in Section 4.4.1. We also correctly determined that the scatterer is nonabsorbing. Our implementation of linear sampling did a good job of estimating the boundary of the scatterers with the largest index of refraction, but it missed the weak scatterers. To distinguish between weak and strong scatterers one must, to some degree, estimate the (relative) index of refraction of the scatterers. This, however, comes at the cost of more data.

4.5 Current Research

The methods we have reviewed are not exhaustive. There are numerous variations and alternative strategies. Current research is tending toward meta-algorithms that use different techniques in concert in order to progressively tease more information out of the data. At the same time, these and other methods have made it possible to do imaging in increasingly diverse settings. Questions such as what constitutes an image and what features allow one to discriminate one object from another are fundamental to the science of imaging. In many cases specific knowledge about a very special case can allow for easy discrimination, however this likely does not generalize. The methods we illustrated here are applications of general principles that can be applied in a wide variety of settings. Research on extending these principles to other physical applications is ongoing. What will not change about these methods is the constant interplay between computational experimentation and analysis. The seeds of discovery are planted with simple tools that generate wonder. We leave the reader with two such tools that are used in Exercise 8 for this chapter, in Chapter 9 of this book.

4.5.1 Starter Code: Obstacle Generation

Below is a listing of *Matlab* code for constructing the kite-shaped object shown in Figure 9.1(a).

```
function [bdy_mat,dbdy_mat]=...
        Make_phantom(theta_res)

% Parameters:
theta_res=240;
objrot=0;

%---------------------------------------------
% Parametric grid generation:
%---------------------------------------------
h=2*pi/(theta_res-1);
t_vec=[0:h:2*pi];
rot_mat =...
 [cos(objrot) -sin(objrot); sin(objrot) cos(objrot)];
bdy_mat=zeros(2,theta_res);
bdy2_mat=zeros(2,theta_res);
dbdy_mat = bdy_mat;

%------------------
% Kite
%------------------
% Boundary:
bdy_mat(1,:)  =  -(cos(t_vec) + 0.65 * cos(2*t_vec) - 0.65);
bdy_mat(2,:)  =  1.5 * sin(t_vec);

% Normal derivative:
% In order to get the correct unit outward normal to the kite-
% shaped obstacle, we have to multiply the derivative by -1.
% The peculiarity is due to the way it is parameterized.
dbdy_mat(1,:) = -(sin(t_vec) + 2*.65*sin(2*t_vec));
dbdy_mat(2,:) = -1.5*cos(t_vec);

figure(1)
plot3(bdy_mat(1,:),bdy_mat(2,:),...
  10*ones(size(bdy_mat(1,:))),'*k')
axis([-5 5 -5 5]) view(2)
title('Obstacle')
```

4.5.2 Starter Code: Far Field Generation

Below is a listing of *Matlab* code for generating the far field data shown in Figure 9.1(b). You will need to change the parameter settings in this code to generate the data shown in Figure 9.1(b).

```
% PARAMETERS:
kappa=10;  % wavenumber
nff=128; % number of far field measurements
n_inc = 128; % number of incident fields
apang = pi; % aperture angle:  pi=full aperture.

% r*_mat are matrices that keep track of the distances
% between the source points, y=(y1,y2), and the
% integration points, x=(x1,x2), on the boundary of the
% scatterer.
% Note that these are parameterized by theta_res
% points on -pi to pi.
% dx*_mat are the matrices of normal derivatives to the
% boundary.
% The following involves a "regularization" of the
% point source, which has a singularity at x=y.
% A more sophisticated numerical quadrature would
% be appropriate for applications that require high accuracy,
% but for the purposes of this exercise, our rough approach
% is very effective.

% Matrix of differences for the kernel
tmp_vec = ones(theta_res,1);
x1_mat=tmp_vec*bdy_mat(1,:);
x2_mat=tmp_vec*bdy_mat(2,:);
dx1_mat=tmp_vec*dbdy_mat(1,:);
dx2_mat=tmp_vec*dbdy_mat(2,:);

min_mat=eps*ones(size(x1_mat));
r1_mat=x1_mat.'-(x1_mat);
r2_mat=x2_mat.'-(x2_mat);
r_mat=max(sqrt(r1_mat.^2 + r2_mat.^2),min_mat);
dr_mat=sqrt(dx1_mat.^2 + dx2_mat.^2);


% Discrete kernel of the integral operators:
S_mat=2*(i/4*besselh(0,1,kappa*r_mat).*dr_mat);
% Hankel function
K_mat=2*(1i*kappa/4*(-dx2_mat.*r1_mat+dx1_mat.*r2_mat)...
  .*(-besselh(1,1,kappa*r_mat))./r_mat);
% The derivative of the Hankel function changes the
% order of the function in K_mat.

A_mat=eye(theta_res)+(2*pi/theta_res)*(K_mat-i*S_mat);

% Incident field at the boundary of the scatterer:
% Incident field has direction d_mat in Cartesian
```

```
% coordinates. The incident directions are not
% perfectly symmetric across the aperture.
h_inc=2*apang/n_inc;
t_inc_vec=[-apang+h_inc/2:h_inc:apang-h_inc/2];

% Incident directions  - Cartesian
d_mat(1,:)=cos(t_inc_vec);
d_mat(2,:)=sin(t_inc_vec);

% Normal to the boundary
d1_mat=bdy_mat(1,:)'*(d_mat(1,:));
d2_mat=bdy_mat(2,:)'*(d_mat(2,:));

b_mat=-exp(i*kappa*(d1_mat+d2_mat));

% Density
phi_mat=A_mat\b_mat;


% Now the far field.
% The measurements are not perfectly symmetric
% across the the aperture.
hff=2*apang/nff;
tff_vec=[-apang+hff/2:hff:apang-hff/2];

% Far field points
ffgrid_mat(1,:)=cos(tff_vec);
ffgrid_mat(2,:)=sin(tff_vec);

% Matrix of differences for the far field kernel
tmp_vec = ones(theta_res,1);
ffx1_mat = (tmp_vec * ffgrid_mat(1,:)).';
ffx2_mat = (tmp_vec * ffgrid_mat(2,:)).';
tmp_vec = ones(nff,1);

x1_mat = tmp_vec * bdy_mat(1,:);
x2_mat = tmp_vec * bdy_mat(2,:);
dx1_mat = tmp_vec * dbdy_mat(1,:);
dx2_mat = tmp_vec * dbdy_mat(2,:);

r1_mat=ffx1_mat.*x1_mat;
r2_mat=ffx2_mat.*x2_mat;
r_mat=r1_mat+r2_mat;
dr_mat=sqrt(dx1_mat.^2 + dx2_mat.^2);

ffM_mat=exp(-i*kappa*r_mat).*dr_mat;
ffL_mat=kappa*(dx2_mat.*ffx1_mat-dx1_mat.*ffx2_mat)...
```

```
        .*exp(-i*kappa*r_mat);
beta=exp(i*pi/4)/sqrt(8*pi*kappa);
ff_mat=beta*(2*pi/theta_res)*(ffL_mat+ffM_mat)*phi_mat;

imagesc(real(ff_mat)), colorbar
```

5 Exploring Strange Functions on the Computer

It appears to me that the Metaphysics of Weierstrass's function still hides many riddles and I cannot help thinking that entering deeper into the matter will finally lead us to a limit of our intellect, similar to the bound drawn by the concepts of force and matter in Mechanics. These functions seem to me, to say it briefly, to impose separations, not, like the rational numbers, in the unboundedly small, but in the infinitely small.[1]

—Paul du Bois-Reymond, 1875 [121]

5.1 What Is "Strange"?

Every computer algebra system has built-in routines for representation, computation, manipulation, and display of elementary and less-elementary functions of analysis, number theory, or probability. Typically, these are smooth functions since often they are solutions of differential equations or are otherwise defined in a similarly analytical way. It is therefore no surprise that many of these techniques do not extend to nonsmooth (*strange*) functions without such convenient differential equations, integral representations, or Taylor series. In this chapter we want to show that even such strange functions can be explored on the computer and useful theorems about them can be discovered. By doing this, we will provide another illustration of our experimental mathodology as expressed in Section 1.5. In fact, a condensation of the eight roles of computation given there to two main points could read as follows: In experimental mathematics, we try to use the computer to

1. generate and test hypotheses by systematic computation, and
2. find paths to a proof of these hypotheses by a mixture of inspired computation and mathematical insight.

[1] *"Noch manches Rätsel scheint mir die Metaphysik der* Weierstrass*schen Functionen zu bergen, und ich kann mich des Gedankens nicht erwehren, dass hier tieferes Eindringen schliesslich vor eine Grenze unseres Intellects führen wird, ähnlich der in der Mechanik durch die Begriffe Kraft und Materie gezogenen. Diese Functionen scheinen mir, um es kurz zu sagen, räumliche Trennungen zu setzen nicht wie die Rationalzahlen im Unbegrenztkleinen, sondern im Unendlichkleinen."*

We will demonstrate these two points on two classes of examples: certain nowhere differentiable functions and certain probability distribution functions that may or may not be singular.

5.2 Nowhere Differentiable Functions

The first example of a continuous, nowhere differentiable function that became widely known is due to Karl Weierstrass. Weierstrass introduced his example in a talk held at the Akademie der Wissenschaften in Berlin, in 1872 [277]; the function was first published by Paul du Bois-Reymond in 1875 [121]. Weierstrass proved that the continuous function

$$C_{a,b}(x) \;:=\; \sum_{n=0}^{\infty} a^n \cos\left(b^n \cdot 2\pi x\right),$$

where $0 < a < 1$ and $b \in 2\mathbb{N}+1$, nowhere has a finite or infinite derivative if $a \cdot b > 1 + \frac{3}{2}\pi$. Figure 5.1 shows an approximation to $C_{0.9,7}$ (the series evaluated to 60 terms at the points $i/(4 \cdot 7^n)$ for $n = 4$).

Until the publication of Weierstrass's example, nineteenth-century mathematicians had been of divided opinions whether such a continuous, nowhere differentiable (cnd) function could exist. Although this question was now answered once and for all by Weierstrass, analysts continued to be fascinated by the Weierstrass example and by cnd functions in general (as is evidenced by the quote that introduces this chapter). Other, sometimes simpler, cnd functions were found; general constructions were given, and of course many aspects of the Weierstrass example itself were investigated. One such aspect is the precise range of the parameters

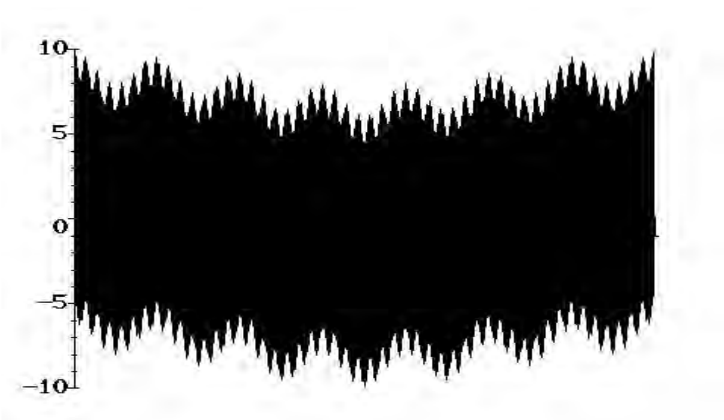


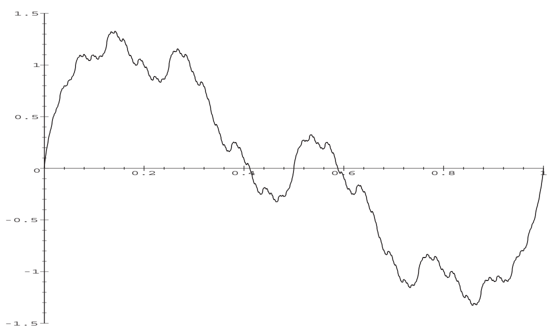
Figure 5.1. Approximation to the Weierstrass function $C_{0.9,7}$.

for which $C_{a,b}$ is nowhere differentiable. It is clear that $C_{a,b}$ is continuously differentiable when $|a|\,b < 1$. But what happens for $1 \leq |a|\,b \leq 1 + \frac{3}{2}\pi$? Or for even integers or reals b? Despite much effort, no real progress on this question was made in the years after Weierstrass. In fact, it took more than forty years until finally, in 1916, G. H. Hardy [158] proved the strongest possible result: Both $C_{a,b}$ and the corresponding sine series

$$S_{a,b}(x) \;:=\; \sum_{n=0}^{\infty} a^n \sin\left(b^n \cdot 2\pi x\right)$$

have no finite derivative anywhere whenever b is a real greater than 1 and $ab \geq 1$. (Hardy also proved that, for small values of $ab \geq 1$, the functions can have infinite derivatives.) This settled the most important questions. However, Hardy's methods are not easy. They use results that lie a good deal deeper than the simple question: Is this function, given by a uniformly convergent series, differentiable somewhere?

Therefore, and because of the fascination many mathematicians feel for such pathological but beautiful objects, research into the Weierstrass functions and into cnd functions in general has continued and continues until today. Several approaches to the Weierstrass functions have been proposed: putting them, for example, into the context of lacunary Fourier series [139, 174], almost periodic



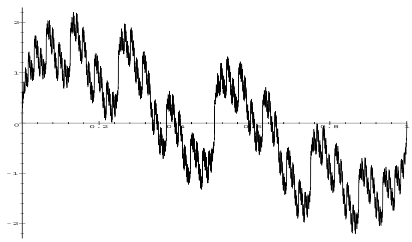


Figure 5.2. The Weierstrass functions $S_{1/2,2}$ (top) and $S_{3/4,2}$ (bottom).

functions [162, 163], functional equations [143, 144], or treating them in their own right (leading to short proofs of nondifferentiability in [30, 38]). Here we will report on the functional equations approach, since it leads to a simple proof of nondifferentiability that can be applied to larger classes of functions and since some key discoveries can be made on the computer. This approach works for integer values of b (a case that is usually investigated separately from the case of arbitrary real b since it employs different, simpler methods), and for didactic reasons we will restrict the discussion to the case $b = 2$ (the inclusion of higher integer values of b would afford more formalism without corresponding gain) and to the function

$$S_{a,2} = \sum_{n=0}^{\infty} a^n \sin\left(2^n \cdot 2\pi x\right)$$

as shown in Figure 5.2 for $a = \frac{1}{2}$ and $a = \frac{3}{4}$. Finally, because of periodicity, it makes sense to restrict our attention to functions defined on the interval $[0,1]$.

5.2.1 Functional Equations

We do not need computers to find promising functional equations for the Weierstrass functions. In fact, it has been known for a long time and is easy to verify that $S_{a,2}$ satisfies

$$S_{a,2}\left(\frac{x}{2}\right) = a S_{a,2}(x) + \sin(\pi x)$$

for all $x \in [0,1]$. In words: The function, taken on $\left[0, \frac{1}{2}\right]$, consists of a rescaled version of itself plus a sine wave.

Unfortunately, this functional equation alone is not sufficient to characterize the Weierstrass function on the interval $[0,1]$. There are many continuous functions, among them almost everywhere (a. e.) differentiable functions, which satisfy the same functional equation on $[0,1]$. Thus, we cannot expect to infer interesting theorems about the Weierstrass function from this functional equation alone. We therefore attempt to add a second functional equation such that the two equations together hopefully are characteristic of the Weierstrass function. Many choices for this second functional equation are possible, of course, but it will turn out that the most natural idea is to replace the term $\frac{x}{2}$ in the functional equation by $\frac{x+1}{2}$, i.e., to take the function not on the first half of the unit interval, but on the second half. This leads to

$$S_{a,2}\left(\frac{x+1}{2}\right) = a S_{a,2}(x) - \sin(\pi x)$$

for all $x \in [0,1]$, also easily verified.

Are these two functional equations together characteristic for the Weierstrass function? To answer this question, we consider functional equations of this type in general. For given constants $|a_0|, |a_1| < 1$ and given *perturbation* functions $g_0, g_1 : [0,1] \to \mathbb{R}$, consider the system consisting of the two functional equations,

$$f\left(\frac{x}{2}\right) = a_0 f(x) + g_0(x), \tag{5.1}$$

$$f\left(\frac{x+1}{2}\right) = a_1 f(x) + g_1(x), \tag{5.2}$$

for unknown $f : [0,1] \to \mathbb{R}$. Special cases of such functional equations have been investigated by G. de Rham in the 1950s [115, 116].

Generalizing in this way makes sense because it turns out that many other strange functions besides the Weierstrass sine series $S_{a,2}$ can be found to satisfy such a system. It is, for example, immediate that the Weierstrass cosine series $C_{a,2}$ solves such a system if g_0, g_1 are chosen as $\pm\cos(\pi x)$. Another example is the so-called Takagi function, after the Japanese mathematician Teiji Takagi, who introduced this function in 1903 [268]. It is defined, for $|a| < 1$, as the series

$$T_a(x) := \sum_{n=0}^{\infty} a^n \, d\,(2^n x),$$

where d is the 1-periodic, saw-tooth function $d(x) := \operatorname{dist}(x, \mathbb{Z})$. The Takagi function (see Figure 5.3 for $a = \frac{1}{2}$ and $a = \frac{3}{4}$) is nondifferentiable for $\frac{1}{2} \le |a| < 1$ and is sometimes considered the simplest cnd function possible; therefore, it (or a variant) is often given as an example in introductory texts. It is again easy to check that this function satisfies the system (5.1)–(5.2) on $[0,1]$ with $a_0 = a_1 = a$, $g_0(x) = \frac{x}{2}$, and $g_1(x) = \frac{1-x}{2}$. More examples of cnd solutions of (5.1)–(5.2) with simple (differentiable) perturbation functions are given in [143, 144].

Now assume that f solves (5.1)–(5.2). Exploring, we find that if we put $x = 0$ into (5.1), then we get that necessarily

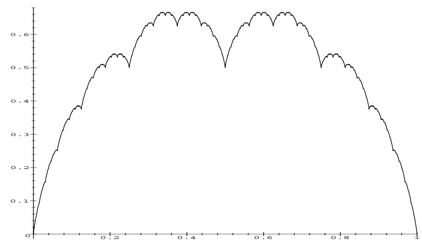
$$f(0) = \frac{g_0(0)}{1 - a_0}.$$

Similarly, from (5.2) with $x = 1$, we get that

$$f(1) = \frac{g_1(1)}{1 - a_1}.$$

This can be continued. Putting $x = 1$ into (5.1), we get

$$f\left(\frac{1}{2}\right) = a_0 f(1) + g_0(1) = a_0 \frac{g_1(1)}{1 - a_1} + g_0(1), \tag{5.3}$$



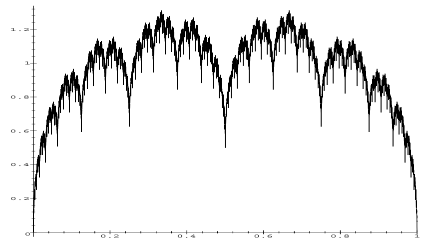


Figure 5.3. The Takagi functions $T_{1/2}$ (top) and $T_{3/4}$ (bottom).

and putting $x = 0$ into (5.2), we get

$$f\left(\frac{1}{2}\right) = a_1 f(0) + g_1(0) = a_1 \frac{g_0(0)}{1-a_0} + g_1(0). \tag{5.4}$$

Thus, if f solves (5.1)–(5.2), then the expressions in (5.3) and (5.4) must be equal. Therefore the condition

$$a_0 \frac{g_1(1)}{1-a_1} + g_0(1) = a_1 \frac{g_0(0)}{1-a_0} + g_1(0) \tag{5.5}$$

must be satisfied if the system (5.1)–(5.2) has a solution.

We can now continue to compute values of the solution f at other points x, using already computed values recursively. Using the value $f\left(\frac{1}{2}\right)$, we get $f\left(\frac{1}{4}\right) = a_0 f\left(\frac{1}{2}\right) + g_0\left(\frac{1}{2}\right)$ and $f\left(\frac{3}{4}\right) = a_1 f\left(\frac{1}{2}\right) + g_1\left(\frac{1}{2}\right)$. From this, we can then compute $f\left(\frac{1}{8}\right), f\left(\frac{3}{8}\right), f\left(\frac{5}{8}\right), f\left(\frac{7}{8}\right)$, $f\left(\frac{2i+1}{16}\right)$, and so on. In this way, we see that the functional equations fix the values of f at all the dyadic rationals $\frac{i}{2^n}$. Since these are dense in $[0,1]$, we see that if there is a continuous solution of (5.1)–(5.2), then it must be unique. By closer inspection of this argument, we are now led to the following theorem, which says that the condition (5.5) above is not only necessary for existence of a solution, but under natural conditions also sufficient.

Theorem 5.1. *If the perturbation functions g_0, g_1 are continuous and condition (5.5) is satisfied, then the system (5.1)–(5.2) has a unique continuous solution.*

Having realized that this theorem holds, it is now in fact not difficult to prove the theorem directly, e.g., with the use of Banach's fixed point theorem. Just define an operator T as mapping f into the function,

$$(Tf)(x) \;=\; \begin{cases} a_0 f(2x) + g_0(2x) & \text{for } x \in [0, \frac{1}{2}], \\ a_1 f(2x-1) + g_1(2x-1) & \text{for } x \in [\frac{1}{2}, 1], \end{cases}$$

and check that T satisfies the assumptions of Banach's theorem with a subset of $(C[0,1], \|\cdot\|_\infty)$ as the Banach space. It also turns out (but is less enlightening) that the theorem can be derived as a special case of theorems on fractal interpolation functions [32].

It is interesting to visualize the recursive procedure to compute values of the solution at the dyadic rationals, described above, on the computer. In the first step, we compute $f(0)$ and $f(1)$ and connect these points by a straight line in the x,y-plane. In the second step, we compute from these the value $f\left(\frac{1}{2}\right)$ and again connect the three known points on the graph of f by straight lines. We repeat this with $f\left(\frac{1}{4}\right)$ and $f\left(\frac{3}{4}\right)$ in the next step, then $f\left(\frac{1}{8}\right), f\left(\frac{3}{8}\right), f\left(\frac{5}{8}\right), f\left(\frac{7}{8}\right)$, and so on. This leads to a sequence of piecewise affine approximations $f^{(n)}$ of f, where $f^{(n)}$ equals f on the dyadic rationals $\frac{i}{2^n}$; see Figure 5.4 (left).

So far, this may look straightforward, but it is already a big step towards a new understanding of the Weierstrass function. The next step now is an insight: the insight to look at the data in a different way that will in fact turn out to be essential for the development of what follows. Thus, a general rule about experimental mathematics is confirmed once more: Being able to compute and draw quickly is not sufficient for gaining new insight; necessary is an active experimenter's mind, interacting with the results and figures and adding ideas to the mix.

In this case, the idea is not only to look at how the approximations approach the solution f, but also to ask oneself what is added in each step. Thus, on the right-hand side of Figure 5.4, we see the differences $f_n := f^{(n)} - f^{(n-1)}$. As expected, these are sawtooth functions (remember that $f^{(n)}\left(\frac{i}{2^n}\right) = f^{(n+1)}\left(\frac{i}{2^n}\right) = f\left(\frac{i}{2^n}\right)$). Not expected in such irregular functions as the Weierstrass functions is the visual regularity of the f_n, apparent in Figure 5.4: Each of these differences, especially in the later figures, seems just to consist of two scaled-down copies of its predecessor.

This is interesting! Having discovered such a pattern where none was to be expected, we should pursue this in more depth. Next stop: the library! Have such triangular functions appeared before in the literature?

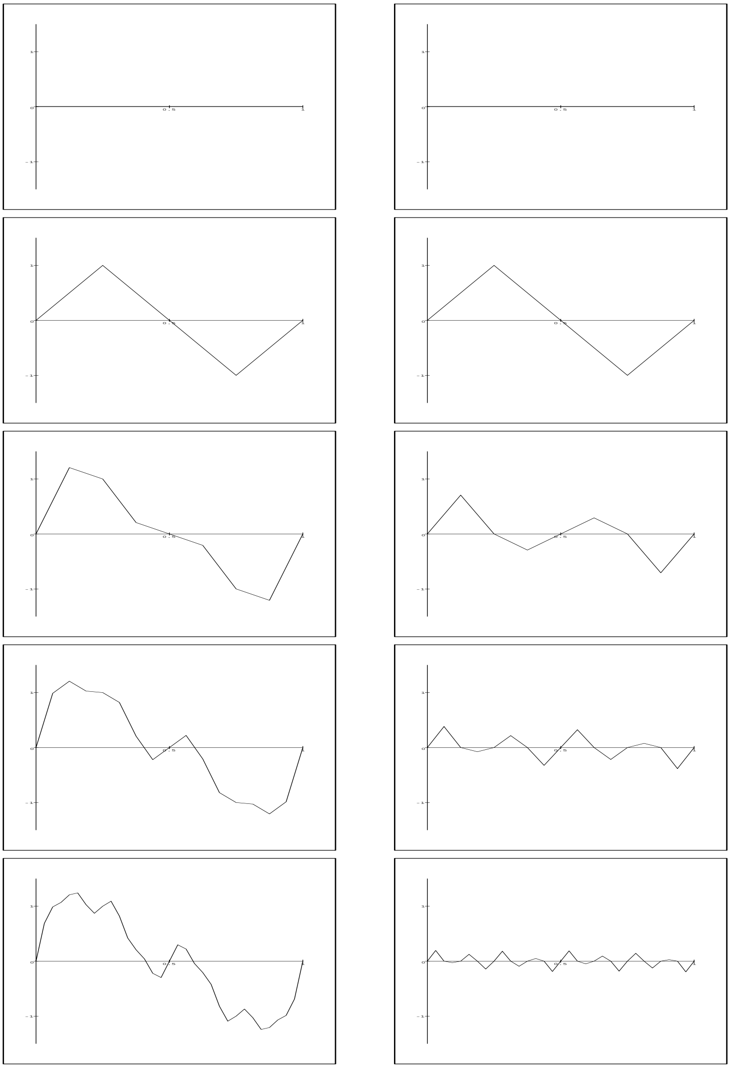


Figure 5.4. Piecewise affine approximations to the Weierstrass function $S_{1/2,2}$.

5.2.2 Schauder Bases

It turns out that indeed these functions have been investigated before, however in a different context. In 1927, J. Schauder [251] introduced the concept of bases in Banach spaces and used these functions as an example. The system of these functions is nowadays called the Schauder basis of $C[0,1]$.

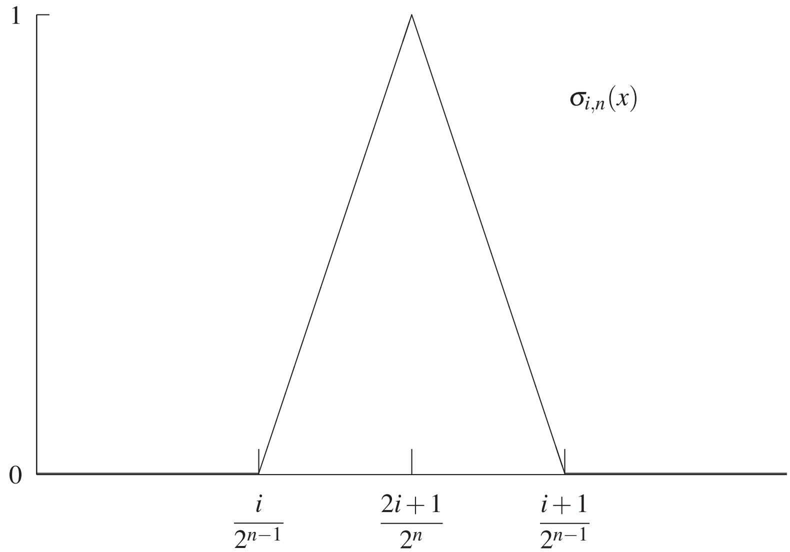


Figure 5.5. An element $\sigma_{i,n}$ of the Schauder basis.

In general, define functions $\sigma_{i,n} : [0,1] \to \mathbb{R}$ by $\sigma_{0,0}(x) = 1-x$, $\sigma_{1,0}(x) = x$, and, for $n \in \mathbb{N}$ and $i = 0, \ldots, 2^{n-1}-1$, define $\sigma_{i,n}$ as the piecewise linear function connecting the points $(0,0)$, $\left(\frac{i}{2^{n-1}}, 0\right)$, $\left(\frac{2i+1}{2^n}, 1\right)$, $\left(\frac{i+1}{2^{n-1}}, 0\right)$, and $(1,0)$; see Figure 5.5.

Then, it is known (and not difficult to prove directly) that every $f \in C[0,1]$ has a unique, uniformly convergent expansion of the form

$$f(x) = \gamma_{0,0}(f)\,\sigma_{0,0}(x) + \gamma_{1,0}(f)\,\sigma_{1,0}(x) + \sum_{n=1}^{\infty} \sum_{i=0}^{2^{n-1}-1} \gamma_{i,n}(f)\,\sigma_{i,n}(x),$$

where the coefficients $\gamma_{i,n}(f)$ are given by

$$\gamma_{0,0}(f) = f(0), \quad \gamma_{1,0}(f) = f(1), \quad \text{and}$$

$$\gamma_{i,n}(f) = f\left(\frac{2i+1}{2^n}\right) - \frac{1}{2} f\left(\frac{i}{2^{n-1}}\right) - \frac{1}{2} f\left(\frac{i+1}{2^{n-1}}\right).$$

For given $f \in C[0,1]$, let

$$f_n(x) := \sum_{i=0}^{2^{n-1}-1} \gamma_{i,n}(f)\,\sigma_{i,n}(x)$$

and

$$f^{(n)}(x) \;:=\; \gamma_{0,0}(f)\,\sigma_{0,0}(x)+\gamma_{1,0}(f)\,\sigma_{1,0}(x)+\sum_{k=1}^{n} f_k(x)$$

and

$$r_n(x) \;:=\; f(x)-f^{(n)}(x) \;=\; \sum_{k=n+1}^{\infty} f_k(x).$$

Note that $r_n(x)=0$ for all dyadic rationals of the form $x=\frac{i}{2^n}$. Remember also that Figure 5.4 shows the $f^{(n)}$'s and f_n's for the Weierstrass function. Thus, the pattern visually discovered in that figure translates into a (recursive) pattern for the $\gamma_{i,n}(f)$'s that we will explore in the next subsection.

For our purposes it is important that differentiability properties of a function can be established by looking at its Schauder coefficients. Statements of this type have apparently been noticed for the first time by G. Faber in 1910 (who used the Schauder basis prior to Schauder but in a different mathematical guise [132,133]). Faber proved the following theorem.

Theorem 5.2. *Assume that $f \in C[0,1]$ has a finite derivative at some point x_0. Then*

$$\lim_{n\to\infty} 2^n \cdot \min\left\{|\gamma_{i,n}(f)| : i=0,\ldots,2^{n-1}-1\right\} \;=\; 0.$$

Proof: Note that if $f'(x_0)$ exists, then

$$f'(x_0) \;=\; \lim_{n\to\infty} \frac{f(v_n)-f(u_n)}{v_n-u_n}$$

for all sequences $(u_n),(v_n) \subseteq [0,1]$ with $u_n \le x_0 \le v_n$ and $u_n < v_n$ and $v_n - u_n \to 0$.

Now, for given $x_0 \in [0,1]$ and $n \in \mathbb{N}$, choose the dyadic rationals u_n, v_n as shown in Figure 5.6 (possibly $x_0 = u_n$ or $x_0 = v_n$ if x_0 is itself a dyadic rational). If $f'(x_0) \in \mathbb{R}$ exists, then

$$\begin{aligned} f'(x_0) &= \lim_{n\to\infty} \frac{f(v_n)-f(u_n)}{v_n-u_n} \\ &= \lim_{n\to\infty} \left[\sum_{k=1}^{n} \frac{f_k(v_n)-f_k(u_n)}{v_n-u_n} + \frac{r_n(v_n)-r_n(u_n)}{v_n-u_n}\right] \\ &= \lim_{n\to\infty} \left[\sum_{k=1}^{n} \pm\delta_{i_k,k}(f)+0\right], \end{aligned}$$

for some sequence i_k, where $\delta_{i,k}(f)$ is the slope of the Schauder triangle $\gamma_{i,k}(f)\,\sigma_{i,k}(x)$ in the expansion of f; thus, $\delta_{i,k}(f)=2^k\gamma_{i,k}(f)$.

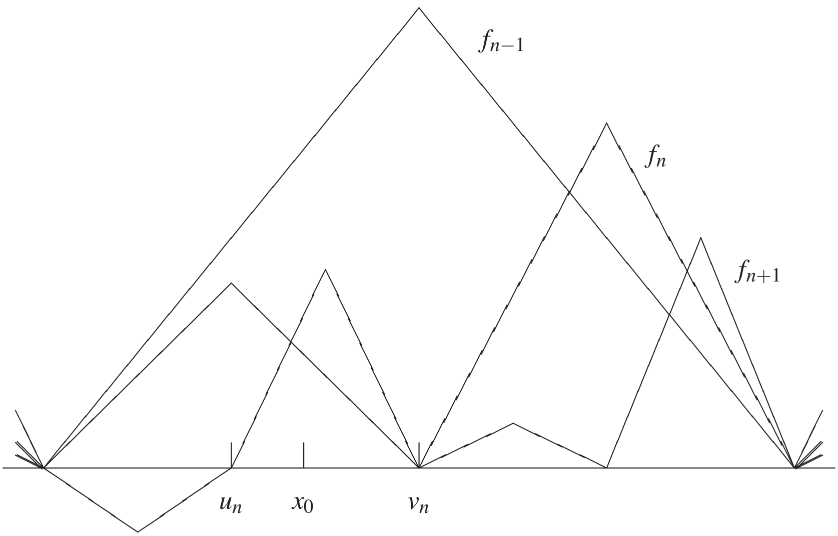


Figure 5.6. Definition of the points u_n and v_n.

This implies that the series $\sum_{k=1}^{\infty} \pm 2^k \gamma_{i_k,k}(f)$ is convergent, hence the summand $\pm 2^k \gamma_{i_k,k}(f)$ necessarily tends to 0, and therefore also

$$\lim_{k\to\infty} 2^k \min_i \left|\gamma_{i,k}(f)\right| = 0. \qquad \square$$

Note that nondifferentiability of the Takagi function T_a for $\frac{1}{2} \leq |a| < 1$, whose Schauder coefficients satisfy $\gamma_{i,n}(T_a) = a^n$, directly follows from this theorem.

5.2.3 Nondifferentiability

By the results of the previous subsection, we can infer differentiability properties of an $f \in C[0,1]$ from its Schauder coefficients. But how can we compute the Schauder coefficients of, say, the Weierstrass functions? In Section 5.2.1 we had already discovered a pattern in these coefficients. With the notation from Section 5.2.2, we can now make this discovery more precise and then use it.

The pattern in fact translates into a recursion formula for the $\gamma_{i,n}(f)$. Since the functional equation was instrumental in discovering the pattern, it is now no surprise that this recursion formula is based on the functional equation as well. Now formulation and proof of the next theorem are straightforward.

Theorem 5.3. *Assume (5.5) and let f be the continuous solution of the system (5.1)–(5.2) with continuous g_0, g_1. Then*
(i) $\gamma_{0,0}(f) = f(0) = \frac{g_0(0)}{1-a_0}$ *and* $\gamma_{1,0}(f) = f(1) = \frac{g_1(1)}{1-a_1}$,

(ii)
$$\begin{aligned}\gamma_{0,1}(f) &= \left(a_1 - \tfrac{1}{2}\right) f(0) - \tfrac{1}{2} f(1) + g_1(0) \\ &= \left(a_0 - \tfrac{1}{2}\right) f(1) - \tfrac{1}{2} f(0) + g_0(1),\end{aligned}$$

(iii)
$$\begin{aligned}\gamma_{i,n+1}(f) &= a_0 \gamma_{i,n}(f) + \gamma_{i,n}(g_0) && \text{for } i = 0, \ldots, 2^{n-1} - 1, \\ \gamma_{i,n+1}(f) &= a_1 \gamma_{i-2^{n-1},n}(f) + \gamma_{i-2^{n-1},n}(g_1) && \text{for } i = 2^{n-1}, \ldots, 2^n - 1.\end{aligned}$$

In consequence, if we let $\delta_{i,n}(f) := 2^n \gamma_{i,n}(f)$, then the recursion step (iii) of the theorem becomes

$$\begin{aligned}\delta_{i,n+1}(f) &= 2a_0 \delta_{i,n}(f) + 2\delta_{i,n}(g_0) && \text{for } i = 0, \ldots, 2^{n-1} - 1, \\ \delta_{i,n+1}(f) &= 2a_1 \delta_{i-2^{n-1},n}(f) + 2\delta_{i-2^{n-1},n}(g_1) && \text{for } i = 2^{n-1}, \ldots, 2^n - 1.\end{aligned}$$

Also, let $\underline{\delta}_n(f) := \min_i |\delta_{i,n}(f)|$. If it can be proved that $\underline{\delta}_n(f) \not\to 0$, then f must be nondifferentiable by Theorem 5.2.

Checking this condition is in fact now relatively easy for the Weierstrass function $f = S_{a,2}$, with the use of the recursion. In Table 5.1 some of the Schauder coefficients and their minimum are listed. The numbers strongly suggest that the minimum indeed does not tend to 0, thus numerically already confirming the function's nondifferentiability. Our task now is to prove this strictly.

The Weierstrass function $f = S_{a,2}$ satisfies the system (5.1)–(5.2) with $a_0 = a_1 = a$ and $g_0(x) = -g_1(x) = \sin(\pi x)$, and thus

$$\delta_{i,n}(g_0) \;=\; -\delta_{i,n}(g_1) \;=\; 2^n \sin\left(\pi \frac{2i+1}{2^n}\right) \cdot \left(1 - \cos \frac{\pi}{2^n}\right).$$

n	$\delta_{0,n}$	$\delta_{1,n}$	$\delta_{2,n}$	$\delta_{3,n}$	$\delta_{4,n}$	$\underline{\delta}_n$
1	0.000000					0.000000
2	4.000000	−4.000000				4.000000
3	5.656854	−2.343146	2.343146	−5.656854		2.343146
4	6.122935	−1.217927	3.468364	−5.190774	5.190774	1.217927
5	6.242890	−0.876323	3.979611	−4.587717	5.793830	0.876323
6	6.273097	−0.786864	4.124884	−4.392211	6.032054	0.786864
7	6.280662	−0.764241	4.162348	−4.340269	6.097976	0.764241
8	6.282555	−0.758569	4.171786	−4.327088	6.114869	0.732594
9	6.283028	−0.757150	4.174150	−4.323780	6.119118	0.704348
10	6.283146	−0.756795	4.174741	−4.322952	6.120182	0.696645
11	6.283175	−0.756707	4.174889	−4.322745	6.120448	0.694677
12	6.283183	−0.756684	4.174926	−4.322693	6.120515	0.693818

Table 5.1. Some Schauder coefficients for $S_{1/2,2}$.

Using the recursion step and estimating, we get the following recursive estimate for the minima $\underline{\delta}_n(f)$:

$$\underline{\delta}_{n+1}(f) \geq 2\,|a| \cdot \underline{\delta}_n(f) - 2^{n+1}\cos\frac{\pi}{2^n}\left(1-\cos\frac{\pi}{2^n}\right).$$

Iterating this and then doing a final estimate, we get

$$\underline{\delta}_{n+k}(f) \geq (2\,|a|)^k\left[\underline{\delta}_n(f) - 2^n\left(1-\cos\frac{\pi}{2^{n-1}}\right)\right].$$

This says that if we can find an index n such that $\underline{\delta}_n(f) > 2^n\left(1-\cos\frac{\pi}{2^{n-1}}\right)$, then it follows that $\underline{\delta}_k(f) \to \infty$ for $k \to \infty$. Such an index can easily be found by computing the δ_n's for $S_{a,2}$ and comparing. We get the following results:

$$\begin{array}{rcll} \underline{\delta}_3\,(S_{a,2}) & = & 8\,|a| - 4\sqrt{2} + 4 & \\ & > & 8 - 4\sqrt{2} = 2^3\left(1-\cos\frac{\pi}{2^2}\right), & \text{for } |a| > \frac{1}{2}; \\ \underline{\delta}_5\,(S_{a,2}) & > & 2^5\left(1-\cos\frac{\pi}{2^4}\right), & \text{for } a = \frac{1}{2}; \\ \underline{\delta}_4\,(S_{a,2}) & > & 2^4\left(1-\cos\frac{\pi}{2^3}\right), & \text{for } a = -\frac{1}{2}. \end{array}$$

Thus the nondifferentiability of the Weierstrass sine series $S_{a,2}$ is completely proved.

Note that this is more than a proof: It is a method. It can be used to examine any nondifferentiable function f that satisfies a system of type (5.1)–(5.2) with simple perturbation functions (simple enough so that the recursion for the Schauder coefficients of f is manageable). Another, rather easy example is given by the Takagi function. Its perturbation functions g_0, g_1 are linear, so their Schauder coefficients vanish. If we did not know that the function was already defined via its Schauder expansion, then the recursion would almost instantly show that the condition of Theorem 5.2 is satisfied.

Another example of a function that can be analyzed by this method is the Weierstrass cosine series $C_{a,2}$. Matters are slightly more complicated, however, since in this case it turns out that $\underline{\delta}_n\,(C_{a,2}) \to 0$ (see Table 5.2). Thus, for this example the method has to be refined a bit, making matters slightly more complicated (but not inherently more difficult). Full details are given in [143, 144]. With such modifications, the Weierstrass cosine series and many other nondifferentiable functions become part of this method, their treatment now being possible in a unified (and quite algebraic, i.e., computational) way. The question of differentiability is essentially reduced to the study of a recursively defined sequence.

Thus, an experimental discovery leads to a significant improvement in our knowledge on nowhere differentiable functions!

n	$\delta_{0,n}$	$\delta_{1,n}$	$\delta_{2,n}$	$\delta_{3,n}$	$\delta_{4,n}$	$\underline{\delta}_n$
1	−4.000000					4.000000
2	−4.000000	−4.000000				4.000000
3	−2.343146	−5.656854	−5.656854	−2.343146		2.343146
4	−1.217927	−5.190774	−6.122935	−3.468364	−3.468364	1.217927
5	−0.614871	−4.679527	−5.781331	−3.348409	−3.588319	0.614871
6	−0.308177	−4.384620	−5.509543	−3.110184	−3.392814	0.308177
7	−0.154182	−4.232107	−5.359982	−2.965015	−3.253435	0.154182
8	−0.077102	−4.155213	−5.283459	−2.889048	−3.178206	0.077102
9	−0.038553	−4.116687	−5.244979	−2.850638	−3.139888	0.038553
10	−0.019277	−4.097413	−5.225712	−2.831379	−3.120641	0.019277
11	−0.009638	−4.087776	−5.216074	−2.821743	−3.111007	0.009638
12	−0.004819	−4.082956	−5.211255	−2.816924	−3.106188	0.004819

Table 5.2. Some Schauder coefficients for $C_{1/2,2}$.

5.3 Bernoulli Convolutions

Consider the discrete probability density on the real line with weight $1/2$ at each of the two points ± 1. The corresponding measure is the so-called Bernoulli measure, denoted $b(X)$. For every $0 < q < 1$, the infinite convolution

$$\mu_q(X) \quad = \quad b(X) * b(X/q) * b(X/q^2) * \cdots \tag{5.6}$$

exists as a weak limit of the finite convolutions. The most basic theorem about these infinite Bernoulli convolutions is due to Jessen and Wintner [173]. They proved that μ_q is always continuous and that it is either absolutely continuous or purely singular. This statement follows from a more general theorem on infinite convolutions of purely discontinuous measures (Theorem 35 in [173]); however, it is not difficult to prove the statement directly with the use of Kolmogoroff's 0-1-law.

The main problem that motivates this section is to decide for which values of the parameter q the measure is singular, and for which q it is absolutely continuous.

This question can be recast in a more real-analytic way by defining the distribution function F_q of μ_q as

$$F_q(t) \quad = \quad \mu_q(-\infty, t] \tag{5.7}$$

and by asking for which q this continuous, increasing function $F_q : \mathbb{R} \to [0,1]$ is singular, and for which q it is absolutely continuous. Note that F_q satisfies $F_q(t) = 0$ for $t < -1/(1-q)$ and $F_q(t) = 1$ for $t > 1/(1-q)$.

A different approach to this function uses the functional equations of type (5.1)–(5.2) that we have discussed in the first section of this chapter. Consider the

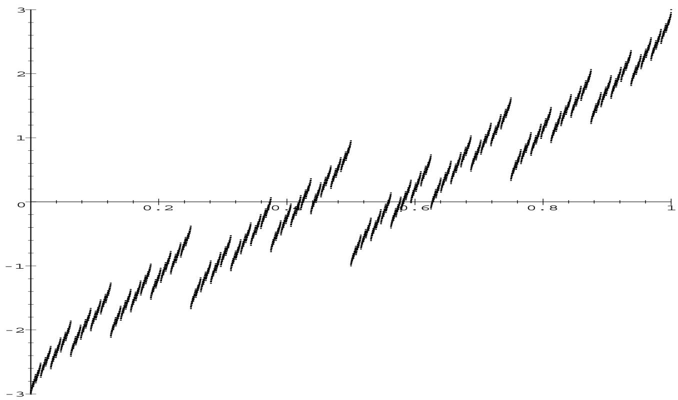


Figure 5.7. Cantor dust (the case $q = 2/3$).

system, for given $0 < q < 1$,

$$s\left(\frac{x}{2}\right) = qs(x) - 1, \quad \text{for } x \in [0,1);$$

$$s\left(\frac{x+1}{2}\right) = qs(x) + 1, \quad \text{for } x \in [0,1].$$

By Banach's fixed point theorem, this system has a unique bounded solution s_q, which moreover can be shown to be discontinuous precisely at the dyadic rationals (it is sometimes called *Cantor dust*; Figure 5.7 shows the case $q = 2/3$).

Then, F_q is the distribution function of s_q, i.e.,

$$F_q(t) = m\{x \in [0,1] \mid s_q(x) \le t\},$$

where m stands for Lebesgue measure.

Approaching the question of singularity vs. absolute continuity experimentally, the probem we set ourselves here is to draw these functions or their derivatives for some well-chosen values of q. However, there is no easy way of computing (let alone graphing) the distribution function or density of a probability measure. One possibility that has been proposed is to generate random numbers which follow this distribution (or an approximation thereof) and count how often these numbers fall into each interval of a partition of $\mathbb{R}$. This method, however, is relatively slow and imprecise.

Thus, we once more need an idea. After the success we had with functional equations in the treatment of nondifferentiable functions, this idea is to use functional equations for the present problem as well.

In fact, it turns out that functional equations can be used to directly define the distribution function F_q: It can be proved that F_q is the only bounded solution of the functional equation

$$F(t) \quad = \quad \frac{1}{2}F\left(\frac{t-1}{q}\right)+\frac{1}{2}F\left(\frac{t+1}{q}\right) \tag{5.8}$$

with $F_q(t) = 0$ for $t < -1/(1-q)$ and $F_q(t) = 1$ for $t > 1/(1-q)$. This can then be used to easily obtain pictures of F_q. Just like the functional equations of type (5.1)–(5.2), (5.8) is also subject to Banach's fixed point theorem; therefore one can easily get pictures of the solution by iteration.

Figure 5.8 shows the respective solutions for $q = 1/3$, $q = 1/2$, and $q = 2/3$. Observationally, F_q is clearly singular for $q = 1/3$ (it is in fact the so-called *Devil's staircase*, a well-known Cantor function, meaning that it is constant on a full-measure set of intervals); it is absolutely continuous (in fact linear on its support) for $q = 1/2$; and it has unclear behavior for $q = 2/3$ (on first glance, however, it looks smooth).

To get a clearer picture of their behavior, one must look more closely at these functions. One possibility for taking such a closer look is to examine the density of F_q. In fact, it can be proved that if F_q is absolutely continuous and thus has a density $F_q' = f_q \in L^1(\mathbb{R})$, then f_q satisfies the functional equation

$$2q\,f(t) \quad = \quad f\left(\frac{t-1}{q}\right)+f\left(\frac{t+1}{q}\right) \tag{5.9}$$

almost everywhere. Vice versa, if this functional equation has a nontrivial L^1-solution f_q, then f_q must be a density of F_q. Therefore, f_q and F_q contain the same information—but f_q may show more structure visually.

If we want to look at the density f_q, we have to understand the functional equation (5.9). This functional equation turns out to be a special case of a much more general class of equations, namely *two-scale difference* (or *scaling*) *equations*. Those are functional equations of the type

$$f(t) \quad = \quad \sum_{n=0}^{N} c_n f(\alpha t - \beta_n) \qquad (t \in \mathbb{R}), \tag{5.10}$$

with $c_n \in \mathbb{C}$, $\beta_n \in \mathbb{R}$, and $\alpha > 1$. They were first discussed by Ingrid Daubechies and Jeffrey C. Lagarias, who proved existence and uniqueness theorems and derived some properties of L^1-solutions [112, 113]. One of their theorems, which

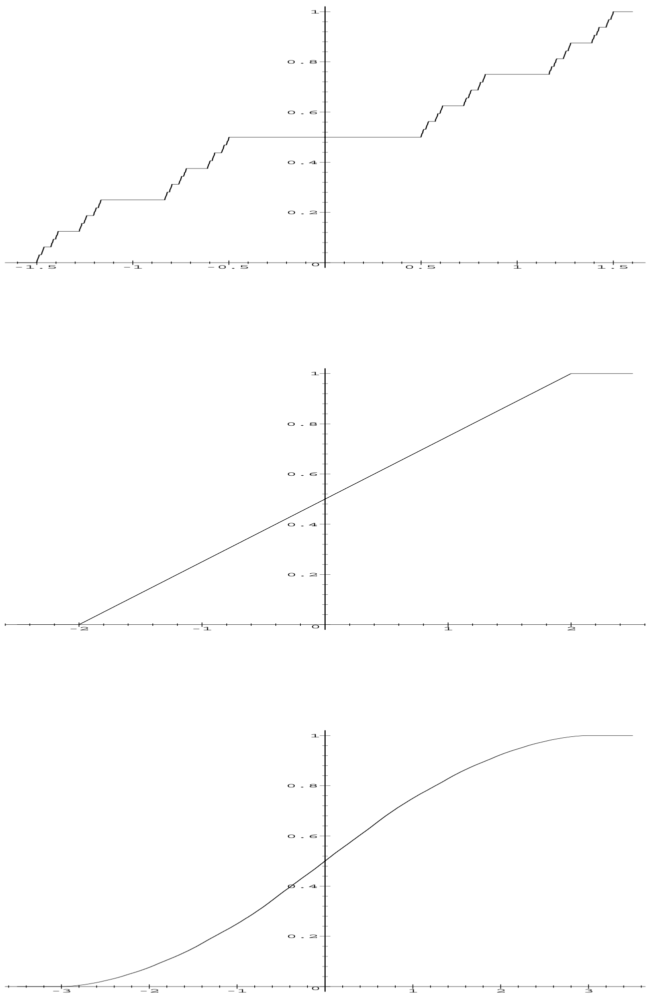


Figure 5.8. The distribution functions for $q = 1/3$ (top; the Devil's staircase), $q = 1/2$ (middle), and $q = 2/3$ (bottom).

we state here in part for the general equation (5.10) and in part for the specific case (5.9), is the following:

Theorem 5.4.

(a) If $\alpha^{-1}(c_0 + \cdots + c_N) = 1$, *then the vector space of* $L^1(\mathbb{R})$*-solutions of (5.10) is at most one-dimensional.*

(b) *If, for given $q \in (0,1)$, equation (5.9) has a nontrivial L^1-solution f_q, then its Fourier transform satisfies $\widehat{f_q}(0) \neq 0$, and is given by*

$$\widehat{f_q}(x) \;=\; \widehat{f_q}(0) \prod_{n=0}^{\infty} \cos(q^n x). \tag{5.11}$$

In particular, for normalization we can assume $\widehat{f_q}(0) = 1$.

(c) *On the other hand, if the right-hand side of (5.11) is the Fourier transform of an L^1-function f_q, then f_q is a solution of (5.9).*

(d) *Any nontrivial L^1-solution of (5.10) is finitely supported. In the case of (5.9), the support of f_q is contained in $[-1/(1-q), 1/(1-q)]$.*

This implies in particular that the question of whether the infinite Bernoulli convolution (5.6) is absolutely continuous is indeed equivalent (as we stated above) to the question of whether (5.9) has a nontrivial L^1-solution. Now what is known about these questions?

It is relatively easy to see that in the case $0 < q < 1/2$ the solution of (5.8) is singular; in fact, it is in this case always a Cantor function: constant on a dense set of intervals. This was first proved by R. Kershner and A. Wintner [178].

It is also easy to see that in the case $q = 1/2$ an L^1-solution of (5.9) can be given explicitly, namely $f_{1/2}(t) = \frac{1}{4}\chi_{[-2,2]}(t)$; this is the density of the function shown in the middle of Figure 5.8. Moreover, this function can be used to construct a solution for every $q = 2^{-1/p}$ where p is an integer, namely

$$f_{2^{-1/p}}(t) = 2^{(p-1)/2} \cdot \left[f_{1/2}(t) * f_{1/2}(2^{1/p}t) * \cdots * f_{1/2}(2^{(p-1)/p}t) \right]. \tag{5.12}$$

This was first noted by Wintner via the Fourier transform [283],

$$\widehat{f}(x) \;=\; \int_{-\infty}^{\infty} f(t)\, e^{-ixt}\, dt.$$

Explicitly, we have

$$\begin{aligned}
\widehat{f_{2^{-1/p}}}(x) \;&=\; \prod_{n=0}^{\infty} \cos(2^{-n/p}x) \;=\; \prod_{m=0}^{\infty} \prod_{k=0}^{p-1} \cos(2^{-(m+k/p)}x) \\
&=\; \widehat{f_{1/2}}(x) \cdot \widehat{f_{1/2}}(2^{-1/p}x) \cdots \widehat{f_{1/2}}(2^{-(p-1)/p}x),
\end{aligned}$$

which is equivalent to (5.12) by the convolution theorem.

Note that the regularity of these solutions $f_{2^{-1/p}}$ increases when p and thus $q = 2^{-1/p}$ increases: $f_{2^{-1/p}} \in C^{p-2}(\mathbb{R})$. From the results given so far, one might therefore surmise that (5.9) would have a nontrivial L^1-solution for every $q \geq 1/2$

with increasing regularity when q increases. This supposition, however, would be wrong, and it came as a surprise when P. Erdős proved in 1939 [125] that there are some values of $1/2 < q < 1$ for which (5.9) does *not* have an L^1-solution, namely, the reciprocals of Pisot numbers. A *Pisot number* is defined as an algebraic integer greater than 1 all of whose algebraic conjugates lie inside the unit disk. The best-known example is the golden mean $\varphi = (\sqrt{5}+1)/2$. The characteristic property of Pisot numbers is that their powers quickly approach integers: If a is a Pisot number, then there exists a θ, $0 < \theta < 1$, such that

$$\operatorname{dist}(a^n, \mathbb{Z}) \leq \theta^n \quad \text{for all } n \in \mathbb{N}. \tag{5.13}$$

Erdős used this property to prove that if $q = 1/a$ for a Pisot number a, then $\limsup_{x\to\infty} \left|\widehat{f_q}(x)\right| > 0$. Thus, in these cases, f_q cannot be in $L^1(\mathbb{R})$, since that would contradict the Riemann-Lebesgue lemma. Erdős's proof uses the Fourier transform $\widehat{f_q}$: Consider, for $N \in \mathbb{N}$,

$$\left|\widehat{f_q}(q^{-N}\pi)\right| = \prod_{n=1}^{\infty} |\cos(q^n\pi)| \cdot \prod_{n=0}^{N-1} \left|\cos(q^{-n}\pi)\right| =: C \cdot p_N,$$

where $C > 0$. Moreover, choose $\theta \neq 1/2$ according to (5.13) and note that

$$\begin{aligned} p_N &= \prod_{\substack{n=0 \\ \theta^n \leq 1/2}}^{N-1} \left|\cos(q^{-n}\pi)\right| \cdot \prod_{\substack{n=0 \\ \theta^n > 1/2}}^{N-1} \left|\cos(q^{-n}\pi)\right| \\ &\geq \prod_{\substack{n=0 \\ \theta^n \leq 1/2}}^{N-1} \cos(\theta^n\pi) \cdot \prod_{\substack{n=0 \\ \theta^n > 1/2}}^{N-1} \left|\cos(q^{-n}\pi)\right| \\ &\geq \prod_{\substack{n=0 \\ \theta^n \leq 1/2}}^{\infty} \cos(\theta^n\pi) \cdot \prod_{\substack{n=0 \\ \theta^n > 1/2}}^{\infty} \left|\cos(q^{-n}\pi)\right| = C' > 0, \end{aligned}$$

independently of N.

Figure 5.9 shows an approximation to the distribution function F_q for $q = (\sqrt{5}-1)/2$. Although this is therefore a function known to be singular, its appearance is almost regular! It is not so much different from the picture for the case $q = 2/3$—whose behavior may now be considered even more unknown than before. This shows the limits of such graphical approaches, unfortunately; however, it is now be even more interesting to examine the behavior of functional equation (5.9).

In 1944, Raphaël Salem [250] showed that the reciprocals of Pisot numbers are the only values of q where $\widehat{f_q}(x)$ does not tend to 0 for $x \to \infty$. In fact, no other $q > 1/2$ are known at all where F_q is singular. (Recently, in [114], "bad behavior," such as unboundedness or nonmembership to L^2, of the density, if it exists,

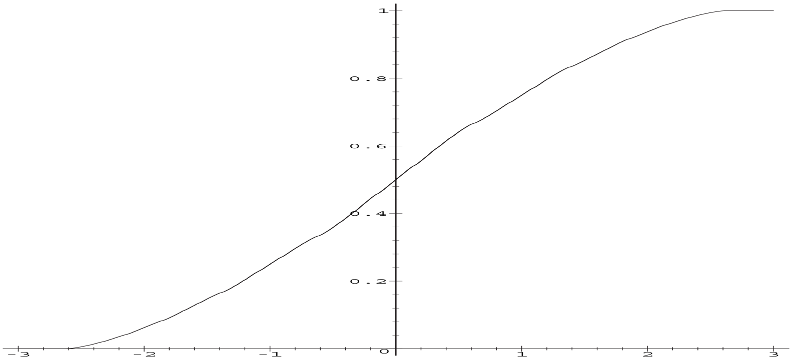


Figure 5.9. The distribution function for $q = (\sqrt{5}-1)/2$, known to be singular.

has been established for certain classes of algebraic numbers.) Conversely, there are only a few values of q where F_q is known to be absolutely continuous: The only such values, besides the roots of $1/2$, are certain algebraic numbers found by A. Garsia in 1962 [140]. He proved that if q^{-1} is algebraic with conjugates outside the unit disk and with minimal polynomial whose constant term is ± 2 (for example, roots of the polynomials $x^{n+p} - x^n - 2$ for $\max\{p,n\} \geq 2$), then F_q is absolutely continuous.

The most recent significant progress in this area was made in 1995 by Boris Solomyak [256], who developed new methods in geometric measure theory that he then used to prove that F_q is in fact absolutely continuous with density in L^2 for *almost every* $q \in [1/2, 1)$. (See also [228] for a simplified proof and [227] for a survey and some newer results.)

Thus, the set of $q \in [1/2, 1)$ with absolutely continuous F_q has measure $1/2$, but does not equal the whole interval. Which numbers are in this set, which are not? Apart from the results cited above, nothing specific is known; in particular, membership to this set has been decided only for some algebraic numbers, not for any rational ones, especially not for $q = 2/3$. The behavior of $F_{2/3}$ is still unknown.

Our goal now is to generate drawings of the functions F_q, or rather, since more structure is visible, of their densities f_q, just to obtain a better visual feeling for their properties. Interestingly, drawing good approximations to these functions is not easy or immediate. It turns out that use of the functional equation appears to be a good way to generate pictures.

In fact, define a map B_q, mapping the set $\mathscr{D}$ of L^1-functions f with support in $[-1/(1-q), 1/(1-q)]$ and with $\widehat{f}(0) = 1$ into itself, by

$$(B_q f)(t) = \frac{1}{2q}\left(f\left(\frac{t-1}{q}\right) + f\left(\frac{t+1}{q}\right)\right) \quad \text{for } t \in \mathbb{R}.$$

One can picture the action of the operator B_q on some $f \in \mathscr{D}$ as putting two rescaled copies of f into the two corners of $[-1/(1-q), 1/(1-q)]$ and adding them.

Now note that the fixed points of B_q are the solutions of (5.9) and that B_q is nonexpansive. Therefore, one may have hope that, by iterating the operator, it may be possible to approximate the solution. Explicitly, we are interested in the iteration

$$\begin{aligned} f^{(0)} \in \mathscr{D} &:= \left\{ f \in L^1(\mathbb{R}) : \operatorname{supp} f \subseteq \left[-\tfrac{1}{1-q}, \tfrac{1}{1-q} \right], \widehat{f}(0) = 1 \right\}, \\ f^{(n)} &:= B_q f^{(n-1)} \text{ for } n \in \mathbb{N}. \end{aligned} \tag{5.14}$$

Since B_q is continuous, it is clear that if a sequence of iterates $B_q^n f^{(0)}$ converges in $L^1(\mathbb{R})$ for some initial function $f^{(0)} \in \mathscr{D}$, then the limit will be a fixed point of B_q. Unfortunately, no general proof of convergence is known, even under the assumption that a fixed point exists. Under this assumption, it is, however, possible to prove a weaker result, namely convergence in the mean:

Theorem 5.5. *If a solution $f_q \in L^1(\mathbb{R})$ with $\widehat{f_q}(0) = 1$ of (5.9) exists, then for every initial function $f^{(0)} \in \mathscr{D}$, we have*

$$\lim_{n\to\infty} \left\| \frac{1}{n} \sum_{k=0}^{n-1} B_q^k f^{(0)} - f_q \right\|_1 = 0.$$

This theorem follows from properties of Markov operators [193] and from a result by Mauldin and Simon [210], showing that, if an L^1-density f_q exists, then it must be positive almost everywhere on its support.

Thus to summarize:

Theorem 5.6. *If the iteration (5.14) converges in $L_1(\mathbb{R})$ for some $f^{(0)} \in \mathscr{D}$, then the limit is a solution of (5.9). If, on the other hand, (5.9) has a solution $f_q \in \mathscr{D}$, then the iteration (5.14) converges in the mean to f_q for every $f^{(0)} \in \mathscr{D}$.*

It is not known (but would be interesting to find out) whether *in the mean* can be dropped in the preceding theorem. Of course, even without knowing whether the iteration converges in the case a solution exists, we can still do the iteration and look at the result. If the iteration *seems* to converge, then we can conjecture existence of a solution. Thus, we are in the same situation as in the previous chapter: The settings in which the methods can be mathematically proven to work are far fewer than those in which they have been computationally demonstrated and thus conjectured to work, but we use them nonetheless.

Regarding the actual computation, note the following. The iterate $f^{(n)} := B_q^n f^{(0)}$ can be expressed explicitly: Let $S_n := \{\pm 1 \pm q \pm q^2 \pm \cdots \pm q^{n-1}\}$. Then

$$(B_q^n f^{(0)})(t) = \frac{1}{(2q)^n} \sum_{s \in S_n} f^{(0)}\left(\frac{t+s}{q^n}\right).$$

The most natural choice for $f^{(0)}$ in this context seems to be

$$f^{(0)} := \frac{1-q}{2} \chi_{[-\frac{1}{(1-q)}, \frac{1}{(1-q)}]}.$$

Then we get: If the limit

$$\lim_{n\to\infty} \frac{1-q}{2\cdot(2q)^n} \sum_{s \in S_n} \chi_{[-\frac{q^n}{(1-q)}-s, \frac{q^n}{(1-q)}-s]} \tag{5.15}$$

exists in $L^1(\mathbb{R})$, then it is the solution in $\mathscr{D}$ of (5.9).

Thus, we now have two different methods to approximate and graph solutions to (5.9): either by iterating B_q or by directly plotting the function in (5.15) for some n. Interestingly, a mixture of both methods seems to work best with respect to computing time, dramatically better, in fact, than either of the two methods alone. The trick is to first compute an approximation by (5.15) and then to use this as a starting function for the iteration.

Figures 5.10 and 5.11 have been computed in this way. They show the indicated iterates, where the nth iterate is defined as $B_q^n f^{(0)}$ with, as above,

$$f^{(0)} := \frac{1-q}{2} \chi_{[-\frac{1}{(1-q)}, \frac{1}{(1-q)}]}.$$

Each function is evaluated at $2^{13}+1$ points, equidistantly spanning the interval $[-1/(1-q), 1/(1-q)]$. In the left-hand columns, the evaluated points $(t, f(t))$ are connected by lines (presupposing continuity); in the right-hand columns, they are just marked by dots. The pictures show how regularity of the solutions (if they exist) generally increases with q, but with exceptions.

For $q = 1/2$, $q = \sqrt{1/2}$, and $q = 3/4$, convergence of the iteration seems relatively clear from the pictures. The picture for $q = 1/2$ is only there to provide an anchor; in this case our $f^{(0)}$ is already the fixed point. The picture for $q = \sqrt{1/2}$ approximates the solution given by (5.12). Note, however, that the approximation was computed by iterating B_q with a step function as starting point. Thus, the picture clearly shows convergence of this iteration, even without taking the mean. For $q = 3/4$, the iteration seems to behave in exactly the same manner, with a continuous limit function.

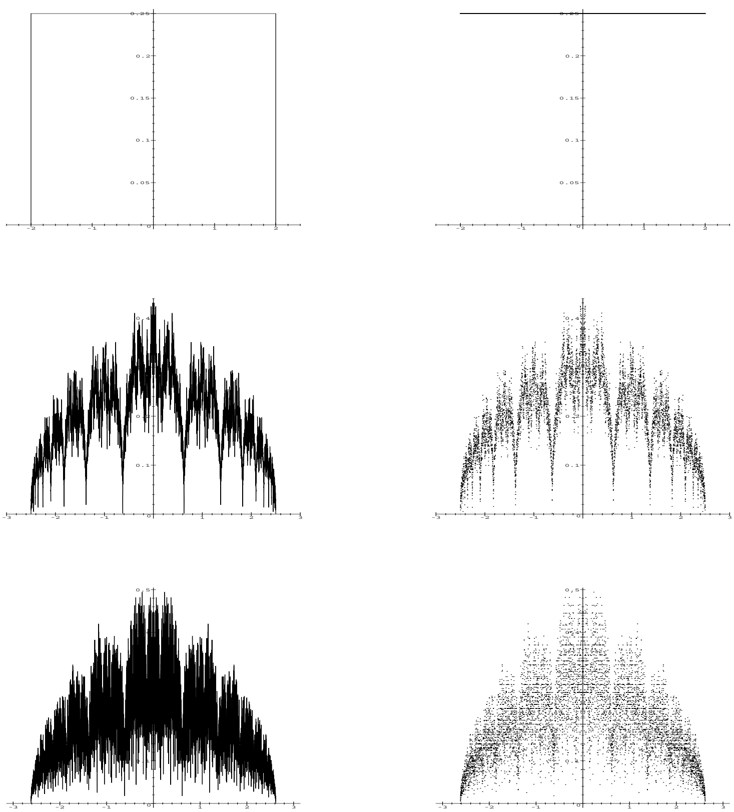


Figure 5.10. The 26th iterate for $q = 1/2$ (top), $q = 0.6$ (middle), and $q = (\sqrt{5}-1)/2$ (bottom).

For $q = 0.6$, $q = (\sqrt{5}-1)/2$, and $q = 2/3$, the situation seems more complicated. For the golden mean, the iteration cannot converge to any meaningful function, and the figure shows this (but compare Figure 5.1, which shows an approximation to a *continuous* function!). For $q = 0.6$, the figure looks only marginally better, so the situation is unclear: Does the figure show approximation to an L^1-function? Or even to a continuous function? Or is there no L^1-solution in this case? Finally, for $q = 2/3$, the iterate seems to be much closer to a definite, maybe even continuous function that would then be a solution of (5.9).

Thus, investigation of figures such as these leads to experimentally derived conjectures, questions, and ideas for further exploration. We close this chapter with some of those.

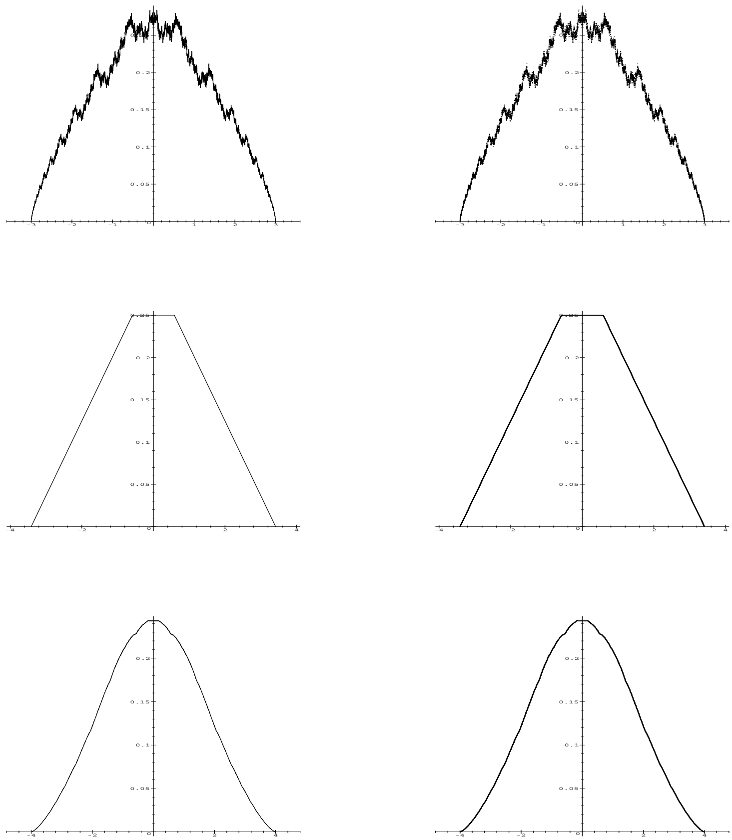


Figure 5.11. The 26th iterate for $q = 2/3$ (top), $q = 1/\sqrt{2}$ (middle), and $q = 3/4$ (bottom).

- **Convergence of the iteration.** Can convergence (pointwise or uniform or in L^1) of the iteration (5.14) with arbitrary or specific $f^{(0)}$ be proved in the case $q = 2^{-1/p}$? The picture indicates this for $p = 2$; for $p = 1$, it is in general not true—for example, for

$$f^{(0)} = \frac{1}{2}\left(1 - \frac{|x|}{2}\right)$$

every point in $[-2,2] \times [0, \frac{1}{2}]$ is then a limit point of some sequence $(x_n, f^{(n)}(x_n))$. Can convergence be proved for other specific values of q (such as $q = 3/4$, as the picture indicates)? Can convergence of the iteration be proved under the sole assumption that a fixed point exists?

- **Boundedness of the iteration.** Can a value of q be identified where the sequence of iterates remains bounded (for arbitrary or specific $f^{(0)}$)? Are there values of q with unbounded iteration? What about the golden mean or any other Pisot number, specifically?

- **Continuity of solutions.** The figures definitely indicate existence of a continuous solution for $q = 3/4$, almost certainly for $q = 2/3$, and maybe for $q = 0.6$. Comparison with Figures 5.2 and 5.3 seems to show a comparable small-scale behavior of the functions shown there for $a = 3/4$ with the iterate shown here for $q = 2/3$. Can some correspondence be established between (5.9) and functional equations of the type (5.1)–(5.2) as investigated there?

- **Existence of a limit function for $q \to 1$.** Is it possible that the solutions f_q (so far they exist), *suitably rescaled,* converge to some well-defined function for $q \to 1$, either pointwise or in some other sense?

6 Random Vectors and Factoring Integers: A Case Study

When the facts change, I change my mind. What do you do, sir?

—John Maynard Keynes[1]

6.1 Learning from Experience

Mathematics is often presented as a fait accompli, a finished result, with little attention being paid to the process of discovery or to the mistakes made, wrong turns taken, etc. However, especially where experimental mathematics is concerned, we can learn a great deal from experience, both our own and that of others. New directions can be suggested by previous mistakes.

In this chapter we will consider as a case study the experiences of one of us supervising undergraduate research, paying particular attention to the role of experiment in introducing students to research at a much earlier stage than is traditional.

For several years, Clemson University has hosted a National Science Foundation supported Research Experiences for Undergraduates program in number theory and combinatorics, supervised jointly by Neil Calkin and Kevin James, with the assistance of two graduate students, Tim Flowers and Shannon Purvis. Each summer nine students are brought to Clemson University for eight weeks to learn what research in mathematics is about. We will focus on the research of two teams, Kim Bowman and Zach Cochran in 2004, and Katie Field, Kristina Little, and Ryan Witko in 2005. At the time of their respective research experiences, all of the undergraduates had completed their junior year, with the exception of Katie Field, who had completed her sophomore year.

Probably the biggest difficulty in having (extremely bright) undergraduates do research is that they lack the breadth and depth of education we traditionally expect of students in graduate studies: This is especially true of students who are not from elite institutions. As a consequence we spend a lot of time in the first few weeks of the REU giving an intensive introduction to the mathematics required to study various problems. In order for the students to be able to get started on research immediately, we try to choose topics having a significant experimental and

[1]Quoted in *The Economist*, December 18, 1999, page 47.

computational component and try to get the participants involved in computing in the first few days of the program.

The students listed above chose to work on projects related to the Quadratic Sieve algorithm for integer factorization.

Throughout this section, n will denote a (large) integer that we wish to factor, and $\mathscr{B} = \{p_1, p_2, \ldots p_k\}$ will denote a finite set of primes, typically the first k primes p for which n is a square (mod p). In practice, k is usually chosen so that $\log k = \sqrt{\log n}$: This choice arises from optimizing the runtime of the sieve.

6.2 Integer Factorization

One of the oldest and most fundamental theorems in mathematics is the fundamental theorem of arithmetic:

> *Every positive integer has a unique factorization into a product of primes.*

An existence theorem, it led to one of the earliest problems in algorithmic mathematics (together with finding solutions to Diophantine equations): given that an integer n *can* be factored, how do we actually *find* integers a, b so that $n = ab$?

Currently the best general purpose factorization algorithms are the General Number Field Sieve (GNFS) and the Quadratic Sieve. Both of these algorithms work by finding distinct square roots of a residue mod n. The questions we discuss here apply to both, but since QS is much simpler, we will restrict our attention to it. Our discussion of the Quadratic Sieve will follow closely that in Pomerance's "A Tale of Two Sieves" [235].

6.2.1 Fermat's Method

The idea of factoring an integer n by finding square roots mod n can be traced back to Fermat. He observed that if we can find integers a and b so that

$$n = a^2 - b^2,$$

then we immediately have the factorization

$$n = (a-b)(a+b).$$

It is clear that, provided that n is odd, the reverse is also true: A factorization $n = (2u+1)(2v+1)$ leads to $n = (u+v+1)^2 - (u-v)^2$, so n can also be written as the difference of two squares.

6.2.2 Kraitchik's Improvement

The first major advance in this direction was by Maurice Kraitchik, who observed that it wasn't necessary that n be a *difference* of two squares: it was enough that

$$a^2 \equiv b^2 \pmod{n}$$

and

$$a \not\equiv \pm b \pmod{n}.$$

Indeed, if $a+b$ and $a-b$ are nonzero $\pmod{n}$, then $n|(a+b)(a-b)$ implies $n|\gcd(a+b,n)\gcd(a-b,n)$, so both $\gcd(a+b,n)$ and $\gcd(a-b,n)$ must be nontrivial factors of n.

The question now is how to find distinct a,b so that $a^2 \equiv b^2 \pmod{n}$. Kraitchik's method was to consider the values taken by $f(x) = x^2 - n$ for values of x slightly larger than $\sqrt{n}$. Since these are all known to be congruent to squares mod n, if we can find a set of these values whose product is a square, then we might be able to use these to factor n.

It is easy to construct an example: To factor the integer $n = 2449$, we observe that $\lceil\sqrt{n}\rceil = 50$: we consider the following squares $\pmod{n}$:

$$\begin{aligned}
50^2 - n &= 3 \times 17, \\
51^2 - n &= 2^3 \times 19, \\
52^2 - n &= 3 \times 5 \times 17, \\
53^2 - n &= 2^3 \times 3^2 \times 5, \\
54^2 - n &= 467, \\
55^2 - n &= 2^6 \times 3^2, \\
56^2 - n &= 3 \times 229, \\
57^2 - n &= 2^5 \times 5^2.
\end{aligned}$$

Rewriting these equations as congruences modulo n, we obtain

$$\begin{aligned}
50^2 &\equiv 3 \times 17 && \pmod{n}, \\
51^2 &\equiv 2^3 \times 19 && \pmod{n}, \\
52^2 &\equiv 3 \times 5 \times 17 && \pmod{n}, \\
53^2 &\equiv 2^3 \times 3^2 \times 5 && \pmod{n}, \\
54^2 &\equiv 467 && \pmod{n}, \\
55^2 &\equiv 2^6 \times 3^2 && \pmod{n}, \\
56^2 &\equiv 3 \times 229 && \pmod{n}, \\
57^2 &\equiv 2^5 \times 5^2 && \pmod{n}.
\end{aligned}$$

Hence, we have

$$(50 \times 52 \times 53 \times 57)^2 \equiv (2^4 \times 3^2 \times 5^2 \times 17)^2 \pmod{n},$$

that is,

$$2424^2 \equiv 657^2 \pmod{2449}.$$

We compute $\gcd(2424+657, 2449) = 79$ and $\gcd(2424-657, 2449) = 31$, and we note that both 31 and 79 are nontrivial factors of n. Indeed, $n = 31 \times 79$. (We should also point out that we could have used $55^2 \equiv (2^3 \times 3)^2 \pmod{2449}$ via Fermat's method.)

6.2.3 Brillhart and Morrison

Brillhart and Morrison [217] found an easy method to systematize the search for a subset whose product is a square: They observed that by considering the vectors of prime exponents in the prime factorizations of $x^2 - n$, a subset had a product which is a square if and only if the corresponding vectors summed to the zero vector (mod 2). In the example above, the fact that $(3 \times 17)(3 \times 5 \times 17)$ $(2^3 \times 3^2 \times 5)(2^5 \times 5^2)$ is a square corresponds to the fact that the vectors of prime exponents sum to a vector all of whose entries are even.

$$\begin{pmatrix}0\\1\\0\\0\\0\\0\\1\end{pmatrix} + \begin{pmatrix}0\\1\\1\\0\\0\\0\\1\end{pmatrix} + \begin{pmatrix}3\\2\\1\\0\\0\\0\\0\end{pmatrix} + \begin{pmatrix}5\\0\\2\\0\\0\\0\\0\end{pmatrix} = \begin{pmatrix}8\\4\\4\\0\\0\\0\\2\end{pmatrix}.$$

Hence, searching for products that are squares is equivalent to finding linear dependencies among the prime exponent vectors considered over the binary field $\mathbb{F}_2$.

A useful and important technical observation here is that if a prime p divides $x^2 - n$, then, since $x^2 \equiv n \pmod{p}$, n must necessarily be a quadratic residue mod p. Hence, any prime for which n is *not* a quadratic residue will always have exponent zero and might as well be ignored in all our computations. In the example above, this explains why the primes 7, 11, and 13 never appear as factors.

Brillhart and Morrison suggested setting a bound B and restricting attention to those x for which $x^2 - n$ factored completely over the set $\mathscr{B}$ of primes (for which n is a quadratic residue) less than B. A value $x^2 - n$ that factors completely over $\mathscr{B}$ will be called $\mathscr{B}$-smooth.

6.2.4 Pomerance and Sieving

A naive implementation of the methods as described above would proceed by attempting to factor x^2-n for each x, checking whether it factors over $\mathscr{B}$, and creating the exponent vector or discarding it as appropriate. Pomerance made the critical observation that this step could be improved immensely by sieving [235]. Rather than factoring one $f(x)=x^2-n$ at a time, he suggested considering the primes p in $\mathscr{B}$ one at a time, and using the observation that if $p|x^2-n$ then $p|(x+p)^2-n$ to extract factors of p from many $f(x)$ values at once. More precisely, find a value x_0 so that $p|f(x_0)$, and then sieve out $x_0, x_0+p, x_0+2p, \ldots$.

The advantage here is that, for each prime in $\mathscr{B}$, the work of determining whether $p|x^2-n$ is shared over all values of x under consideration. The disadvantage is that the method inherently needs the range of x being considered to be fixed in advance. This leads to the following questions:

- How many x do we need to consider to obtain l $\mathscr{B}$-smooth numbers?
- How large does l have to be in order for a set of l $\mathscr{B}$-smooth numbers to have a product which is a square?

If $|\mathscr{B}|=k$, then clearly if we have $k+1$ exponent vectors, each having k coordinates, then the set must be linearly dependent. However, it is possible that the first linear dependency could occur far earlier. Since the Quadratic Sieve is a sieve, in order to obtain the full efficiency of the algorithm, the set of x for which we will attempt to factor x^2-n has to be determined in advance: Adding just a few more x values after the fact is expensive.

6.3 Random Models

We can regard the Quadratic Sieve as taking a range $1,2,\ldots,R$, and for each i in the range setting $x=\lfloor\sqrt{n}\rfloor+i$ and returning either FAIL (if x^2-n doesn't factor over the factor base $\mathscr{B}$) or a vector $\underline{v}_i$, the entries of which are the parities of the exponents of the primes in the factor base in the factorization of x^2-n. Although the vectors $\underline{v}_i$ and the indices for which we get FAIL are deterministic, they are hard to predict and (in a strong sense) look random.

Although most questions in number theory are completely deterministic, it is often possible to obtain insight (and sometimes even theorems) by considering random models that behave similarly to the integers.

Erdős and Kac [126] introduced the idea of probabilistic methods in number theory in 1945. Building on work of Hardy and Ramanujan [161], they showed that the number of prime factors of a randomly chosen large integer, suitably normalized, approximately follows a normal distribution. This led to a host of similar theorems.

As we noted above, the Quadratic Sieve can be viewed as producing a sequence of vectors whose entries are distributed in a quasi-random fashion. If we choose an appropriate probabilistic model, we may be able to predict the behavior of the Quadratic Sieve based on the behavior of the random model.

Of course, this would not prove that the sieve behaves in a particular fashion. However, it would suggest possible parameter choices that could be tested empirically.

We will discuss two different types of models, with various different possibilities for parameters. In each model, vectors will be chosen independently with replacement from the same distribution.

The first model will be vectors chosen uniformly from the set of vectors of weight w (and the generalization of this to vectors with a given distribution of weights). In this chapter, the *weight* of a vector is its number of nonzero entries.

In the second model, vectors will have entries that are chosen independently, but with different probabilities.

6.4 The Main Questions

The main questions now are the following:

- What is the right random model for vectors arising from sieves?
- Given a model for randomly generating vectors in $\mathbb{F}_2^k$, how many vectors do we need to select before we get a linear dependency?

6.4.1 The Constant Weight Model

Let $\omega(m)$ be the number of distinct prime factors of m. Hardy and Ramanujan [161] proved that if $g(m) \to \infty$, then the number l_n of integers m in $\{1,2,3,\ldots,n\}$ for which

$$|\omega(m) - \log\log m| > g(m)(\log\log m)^{1/2}$$

satisfies $l_n = o(n)$.

Less precisely, they showed that almost all numbers m have about $\log\log m$ distinct prime factors and that the probability of differing from this by much more than $(\log\log m)^{1/2}$ tends to 0.

Erdős and Kac [126], in their seminal paper introducing probabilistic number theory, showed that if m is chosen uniformly from $\{1,2,3,\ldots,n\}$, then the distribution of

$$\frac{\omega(m) - \log\log m}{(\log\log m)^{1/2}}$$

converges to the normal distribution as n tends to infinity.

This suggests the following approach to developing a random model for the vectors arising from the sieve: The vectors v_i that are produced by the Quadratic Sieve correspond to numbers in the range $(1,2,3,\ldots n-1)$, so they ought to have about $\log\log n$ distinct prime factors. Furthermore, Canfield, Erdős, and Pomerance [81] showed that, given a bound B, the proportion of B-smooth numbers less than n is about e^{-u}, where $u = \log n/\log B$. Hence for our first model, for each i in the range, we will generate FAIL with probability $1 - e^{-u}$, and with probability e^{-u} we will pick a vector of weight $w = \log\log n$ uniformly from $\mathbb{F}_2^k$. (Recall that in the implementations of the Quadratic Sieve, k is typically chosen so that $\log k \simeq \sqrt{\log n}$: hence $\log\log n \simeq 2\log\log k$.)

6.4.2 The Independent Entries Model

Fix a prime p. Since a random integer chosen uniformly from a large range is divisible by p^e with probability about $1/p^e$, the probability that it is divisible by an odd power of p is

$$\frac{1}{p} - \frac{1}{p^2} + \frac{1}{p^3} - \frac{1}{p^4} + \cdots = \frac{1}{p+1}.$$

Hence, we might choose the following model: Take as the factor base a set $\mathscr{B} = \{p_1, p_2, \ldots, p_k\}$. Each component of the vector $\underline{v}_i$ is chosen uniformly and independently, and the probability that the j component of $\underline{v}_i$ is 1 is

$$\Pr(\underline{v}_i[j] = 1) = \frac{1}{p_j + 1}.$$

As we shall see later, we will want to modify this slightly so that

$$\Pr(\underline{v}_i[j] = 1) = \alpha_j,$$

where α_j will be chosen to take into account some subtle complications.

6.5 Bounds

It is a simple fact from elementary linear algebra that if we have $l \geq k+1$ then any set of l vectors in a vector space of dimension k is linearly dependent. This fact has typically been used in implementations of the Quadratic Sieve to determine a range to be sieved over: Choose an l somewhat larger than k, and use Canfield, Erdős, and Pomerance's estimates on the proportion of smooth numbers to determine the size of range required to produce l $\mathscr{B}$-smooth numbers. If we could determine a bound L, significantly less than k, so that with high probability any L exponent vectors are linearly dependent, then this would improve the runtime of the sieve in the following ways:

1. The sieving stage of the algorithm would need to return fewer $\mathscr{B}$-smooth numbers: This would decrease the runtime.
2. The linear algebra stage of the algorithm would involve finding a linear dependency in a matrix with fewer rows, also decreasing the runtime.
3. It is possible that stopping the algorithm earlier will allow us to use preprocessing on the vectors, which will significantly decrease the size of the linear algebra problem.
4. The change would allow us to optimize the parameters k and $\mathscr{B}$ based on the new runtimes: This might also improve the runtime.

Of these, the sieving stage is likely to be least significant: This stage of the algorithm is easily parallelized, and indeed, the most recent examples of factorization records have been set by parallel implementations.

The matrix stage has more potential: This stage is now becoming the bottleneck for factoring.

The reoptimizing would be necessary to take full advantage of speedups especially in the linear algebra phase.

6.5.1 Upper Bound for the Constant Weight Model

Consider the constant weight $w = w(k)$ model. Recall that we pick l vectors uniformly from the set of vectors of weight w in $\mathbb{F}_2^k$. The probability that a given vector has a 0 in the jth coordinate is $(1 - w/k)$. Since the vectors are chosen independently, the probability that all of the vectors have a zero in the jth coordinate is

$$\left(1 - \frac{w}{k}\right)^l .$$

Hence, if we pick k vectors this way, the expected number of coordinates that are never 1 is about ke^{-w}. Thus, our vectors are contained in a subspace of dimension less than $k(1 - e^{-w})$, and the first linear dependency will probably occur for some $l < k(1 - e^{-w})$. Since we only get information about the expected number of coordinates, we need to use a sharp concentration result to show that the probability that we are not close to the expected value is small. This is technical, but standard and straightforward.

6.5.2 Upper Bound for the $\alpha_j = 1/(p_j+1)$ Model

As is usually the case, similar methods work for the α_j model, but the analysis is rather more delicate and depends on the behavior of each α_j. We recall that in this model we obtain vectors $\underline{v}_i$, which form the rows of a matrix $A = (a_{ij})$, so that

$$\Pr(a_{ij} = 1) = \alpha_j$$

independently. Hence, the probability that column j is empty (i.e., has no 1's) is $(1-\alpha_j)^l$, and in most of the cases we'll be considering, either this will be very small or $(1-\alpha_j)^l \simeq e^{-l\alpha_j}$. Thus, the expected number of nonempty columns $E(C_l)$ is given by

$$E(C_l) = \sum_{j=1}^{k} 1-(1-\alpha_j)^l \simeq \sum_{j=1}^{k} 1-e^{-l\alpha_j}.$$

In the most simplistic model of this type, we take $\alpha_j = 1/(p_j+1)$. We make the reasonable assumption that our factor base contains about half of the primes up to B and that $p_j \sim 2j\log j$. Now it is easy to see that

$$E(C_l) \simeq \sum_{j=1}^{k} \left(1-e^{-l/(p_j+1)}\right). \tag{6.1}$$

If $E(C_l) < l$, then (after again applying an appropriate sharp concentration result) we can conclude that with high probability the vectors $\{\underline{v}_1, \underline{v}_2, \ldots, \underline{v}_l\}$ are linearly dependent.

The sum in (6.1) can be estimated by splitting it into appropriate ranges. A suitable choice of ranges is

(I) $1 \le j \le l/(\log l)^2$

(II) $l/(\log l)^2 < j \le l$

(III) $l < j \le k$.

Since the summands are all at most 1 and we are concerned with the size of the sum relative to l, the contribution of range (I) is negligible. We approximate the second range by an integral, replacing p_j+1 by $2j\log j$. It is then easy to see that the contribution of this range is $O\left(l\frac{\log\log l}{\log l}\right)$. Finally, in region (III), $l/(p_j+1)$ is small, so the summand is approximately $\frac{l}{p_j+1}$. By Merten's theorem (and assuming that about half of the primes are in the sum), the contribution of this region is about $l(\log\log k - \log\log l)/2$. Hence, if $\log\log k - \log\log l < 2$, we have $E(C_l) < l$. Writing $l = k^\delta$, this gives $-\log\delta < 2$, that is, $\delta > e^{-2}$. Hence, if we have many more than k^{1/e^2} vectors in this model, we expect to see linear dependence.

At this point the students investigating the model got very excited, since this would lead to an immense speed-up in the Quadratic Sieve. However, after implementing the Quadratic Sieve, they discovered that the predictions were far too optimistic; this led to a re-examination of the assumptions of the model.

6.5.3 Lower Bounds

Lower bounds for these models are both more difficult and less suggestive of suitable choices of parameters for the sieve. However, we can obtain some results in both choices of model.

Calkin [80] and Balakin, Kolchin, and Khokhlov [29, 185] showed independently that in the case of vectors of fixed constant weight w the following is true:

Theorem 6.1. *There is a constant $\beta = \beta(w)$ so that if $b > \beta$ and $l = l(k) < kb$, then as $k \to \infty$ the probability that a set of l vectors chosen uniformly from the vectors of weight w in $\mathbb{F}_2^k$ is linearly independent tends to 1.*

Essentially this theorem says that we need about βk vectors to obtain a linearly dependent set: Careful analysis shows that

$$\beta(w) \simeq 1 - \frac{e^{-w}}{\log 2}$$

and that, if $w = w(k) \to \infty$ as $k \to \infty$ (and $w < k/2$), then $\beta(w) \to 1$.

How would we discover and prove such a theorem? We want to know how likely it is that a set of vectors is dependent. Can we determine the probability that a given set of vectors sums to the zero vector? This suggests trying a Markov chain approach: Start at the origin and add random vectors of weight w using a transition matrix $T = T_w$ to compute the probability that we end up back at the origin.

Since the transition matrix will have size $2^k \times 2^k$, it is natural to try to use the symmetry of the problem to reduce the complexity. Note that we can do this by grouping together points in $\mathbb{F}_2^k$ by weight. Then the probability T_{ij} of moving from a vector of weight i to a vector of weight j by adding a random vector of weight w is precisely

$$T_{ij} = \frac{\binom{i}{\frac{w+i-j}{2}}\binom{k-i}{\frac{w-i+j}{2}}}{\binom{k}{w}}.$$

(If we have i 1's in a vector, and we flip x of them to 0's and flip $w-x$ of the other 0's to 1's, then we end up with $j = i - x + (w - x)$ 1's as a result; hence,

$x = (w+i-j)/2$.) Using this transition matrix, we can obtain an expression for the probability of a random walk on the hypercube returning to the origin after a given number of steps.

Experimentation in *Maple* now reveals the beautiful fact that the transition matrix T is diagonalizable and that its eigenvalues and eigenvectors have rational entries, which can be expressed in terms of sums of binomial coefficients.[2] Hence, we can write down an expression for $E(2^s)$ that is amenable to analysis, leading to the theorem above.

A key observation now is that this is exactly the probability that a set of vectors sums to zero: If we sum this over all subsets of an l-set of vectors, we obtain the expected number of linear combinations that sum to zero, that is, the expectation $E(2^s)$ of the size of the left null space of the matrix A whose rows are the vectors $\underline{v}_1, \underline{v}_2, \ldots, \underline{v}_l$ (that is, s is the co-rank of A). If $E(2^s)$ is close to 1, then the set $\{\underline{v}_1, \underline{v}_2, \ldots, \underline{v}_l\}$ is likely to be linearly independent. This method works by considering the left null space of A. One can perform a similar calculation, giving exactly the same results, using the right null space of A.

Since we now have upper and lower bounds for the constant weight vector models, it makes sense to ask whether there is a sharp threshold for linear dependence: that is, does there exist a threshold value b_t so that

if $b < b_t$, then $\lim_{n\to\infty} Pr(\text{dependent}) = 0$,
if $b > b_t$, then $\lim_{n\to\infty} Pr(\text{dependent}) = 1$.

This in fact was where Bowman and Cochran started their investigations, generating random binary vectors with exactly three 1's and computing when the set of vectors generated first becomes dependent.

Similar methods, both for the left and the right null space can be applied to the α_j model: In this case the bounds obtained are harder to analyze and, of course, depend on the behavior of the parameters α_j.

6.6 Which Model Is Best?

The constant weight model is easily seen to be inappropriate: The model assumes that the probability that a large prime divides $x^2 - n$ is the same as the probability that a small prime does. Hence, the depressing fact that the lower and upper bounds for the number of vectors required to obtain an independent set with high

[2] It also turns out that the eigenvectors for T_w are independent of w. Hence, for two distinct weights w and w', the matrices T_w and $T_{w'}$ commute. This corresponds to the observation that, if we start with a vector of weight w and add a vector of weight w', the effect is the same as starting with a vector of weight w' and adding a vector of weight w. This is intimately related to the fact that there is an *association scheme*, the *Hamming scheme* here.

probability are both asymptotic to k, the dimension of the space, is irrelevant to the Quadratic Sieve.

The second model, where

$$\Pr(\underline{v}_i[j]=1)=\frac{1}{p_j+1},$$

requires more thought. In this model, the upper bounds on probable linear dependencies occur *far* earlier than k. Indeed, upon proving these bounds the students immediately set to coding up the Quadratic Sieve to see if the behavior occurred in reality. Unfortunately, the tests that they ran suggested that the model was far too optimistic. Indeed, although the model seemed as if it ought to be much better than the constant weight model, it gave results that were much further off!

This led to much head scratching, trying to figure out why a seemingly reasonable model could give results that were so far out of touch with reality.

The key point here is the following: First, the reason that the model is incorrect is that it fails to take into account the fact that we are conditioning on numbers being $\mathscr{B}$-smooth. We will give a simple example in a moment to show how drastically this can change probabilities. The reason that even seemingly small changes can have a large impact on the sieve is that we will end up estimating sums which behave like

$$\sum_{i<x}\frac{1}{i}\simeq\log x$$

instead of

$$\sum_{i<x}\frac{1}{i\log i}\simeq\log\log x.$$

This will mean that a term which can be controlled in the inappropriate model will never be small in the corrected model.

Why can smoothness change things drastically? Consider the following question: What is the probability that a random integer is divisible by 2? If the integer is chosen uniformly from a large interval, then the answer is very close to $1/2$. However, if we choose uniformly from $\mathscr{B}$-smooth numbers less than x, then we see the following:

1. If $\mathscr{B}=\{2\}$, then there are $\lfloor\log_2 x\rfloor+1$ $\mathscr{B}$-smooth numbers up to x, and all but one is divisible by 2. Hence, the probability that a random $\mathscr{B}$-smooth number is even is
$$1-\frac{1}{\lfloor\log_2 x\rfloor+1}.$$
2. If $\mathscr{B}=\{2,3\}$, then the number of $\mathscr{B}$-smooth numbers up to x is equal to the number of nonnegative integer solutions to the inequality
$$i\log 2+j\log 3\le\log x.$$

For large x, this in turn is about equal to the area of the corresponding triangle, namely

$$\frac{1}{2}\frac{\log x}{\log 2}\frac{\log x}{\log 3} = \frac{1}{2}\log_2 x \log_3 x.$$

Now the number of these that are not divisible by 2 is exactly the number of powers of 3 less than x, namely $\lfloor \log_3 x \rfloor + 1$; hence, the probability that a random $\mathscr{B}$-smooth number less than x is even is about

$$1 - \frac{\lfloor \log_3 x \rfloor + 1}{\frac{1}{2}\log_2 x \log_3 x} \simeq 1 - \frac{2}{\log_2 x}.$$

6.6.1 Refining the Model

We wish now to refine the model to compensate for conditioning on $\mathscr{B}$-smoothness. A first attempt at this will proceed by modifying α_j, the probability of divisibility by the jth prime p_j in $\mathscr{B}$. Naively (by which we mean that this is what we actually did and thought correct for several months!), we let B be the largest element of $\mathscr{B}$, fixed a prime $p < B$, and considered the number of B-smooth numbers up to n and the number of B-smooth numbers divisible by p: The second quantity is exactly equal to the number of B-smooth numbers less than n/p. Using Canfield, Erdős, and Pomerance's estimates for the number of B-smooth numbers and estimating some asymptotics, this leads to the following approximation:

$$\Pr(p \text{ divides } m \mid m \text{ is } B\text{-smooth and } \leq n) \simeq \frac{1}{p^{1-\delta}}$$

in which $\delta = \frac{\log u}{\log B}$ and $u = \frac{\log n}{\log B}$. Using the parameters usually chosen for the Quadratic Sieve, this gives $\log B \simeq \log k \simeq \sqrt{\log n}$, so $u \simeq \sqrt{\log n}$ and

$$\delta \simeq \frac{\frac{1}{2}\log\log n}{\log B} \simeq \frac{\log\log k}{\log k}.$$

When p is small, p^δ is very close to 1. However, when, say p is not $o(k)$, which is the case for most primes in $\mathscr{B}$, then

$$p^\delta \simeq \exp\left(\frac{\log p \log\log k}{\log k}\right) \simeq \log k \simeq \log p.$$

Is this model now appropriate? It is rather hard to compare empirical data from the Quadratic Sieve at this stage, because our estimates have been a little careless with constants. However, if our model was inappropriate, and in fact some aspect that we have ignored should be considered and would introduce a factor, say, of $\log\log\log\log n$, would we be able to tell? If we run the Quadratic Sieve on toy problems, say with n about 10^{15}, then $\log\log\log\log n$ is much less than 2: Even $\log\log n \simeq 3.5$ in this range!

However, having realized that there is a problem with conditioning on smoothness, let us now try to take it into account at every stage.

Let $\mathscr{P}$ denote the set of all primes for which n is a quadratic residue (mod p). It is known that this set has relative density about 1/2 in the set of all primes. However, we will mainly be concerned with the small primes in the set (those less than n, say) and much less is known about the number of small primes in the set. In the examples we have studied, $\mathscr{P}$ appears to contain about half the primes in reasonably sized intervals.

Now $\mathscr{B}$ will be the set of primes $\{p_1, p_2, \ldots, p_k\}$ less than B that are contained in the set $\mathscr{P}$. We will write $\mathbb{Z}_{\mathscr{P}}$ for the set of $\mathscr{P}$-smooth numbers and $\mathbb{Z}_{\mathscr{B}}$ for the set of $\mathscr{B}$-smooth numbers.

Now, the probability that the Quadratic Sieve returns a vector rather than FAIL should be about the probability that an integer m chosen uniformly in $\{1, 2, \ldots, n\}$ is $\mathscr{B}$-smooth given that it is $\mathscr{P}$-smooth. This leads to the following natural questions: given a set $\mathscr{P}$ of primes (of relative density 1/2 in the set of all primes) and a finite subset $\mathscr{B}$ of $\mathscr{P}$,

1. what is the number $Z_{\mathscr{P}}(y)$ of $\mathscr{P}$-smooth integers up to y?
2. what is the number $Z_{\mathscr{B}}(y)$ of $\mathscr{B}$-smooth integers up to y?

Then, the probability that $x^2 - n$ returned by the sieve is $\mathscr{B}$-smooth should be about $Z_{\mathscr{B}}(n)/Z_{\mathscr{P}}(n)$. Furthermore, the probability that $x^2 - n$ is divisible by p, given that it is $\mathscr{B}$-smooth, ought to be about $Z_{\mathscr{B}}(n/p)/Z_{\mathscr{B}}(n)$.

Landau [191] and Wirsing [284] have addressed various versions of these questions: In particular, if y is allowed to be arbitrarily large, then Wirsing gave precise asymptotics for the behavior of the function $Z_{\mathscr{P}}(y)$. When $|\mathscr{B}|$ is sufficiently small, $Z_{\mathscr{B}}(y)$ is also easy to estimate. However, in the regions relevant to the sieve, results are harder to obtain. We are interested in the behavior of $Z_{\mathscr{P}}(y)$ when y is somewhat smaller than n and $\mathscr{P}$ is the set of primes for which n is a quadratic residue $\pmod p$. Since $\mathscr{P}$ is defined in terms of n, it seems unlikely that asymptotic results will be possible for values this small. However, there is some hope that the behavior is similar for small values, and since we are primarily interested in heuristics, we will make this assumption.

Theorem 6.2 (Wirsing). *Let $\mathscr{P}$ be a set of primes for which there exist constants δ and K so that*

$$\sum_{p<y, p\in\mathscr{P}} 1 \sim \delta \frac{y}{\log y}$$

and

$$\prod_{p<y, p\in\mathscr{P}} \left(1 - \frac{1}{p-1}\right) \sim K(\log y)^{\delta}.$$

Then

$$Z_{\mathscr{P}}(y) \sim \frac{\delta K e^{-\gamma\delta}}{\Gamma(\delta+1)} \frac{y}{(\log y)^{1-\delta}}$$

(in which γ is the Euler-Mascheroni constant and Γ is the Gamma function).

Following the heuristics suggested by the previous section, it seems reasonable to assume that the probability α_j that $p_j | x^2 - n$, given that $x^2 - n$ is $\mathscr{B}$-smooth, should be about $c \log p_j / p_j$ for some constant c.

Since we also have the heuristic that about half the primes are in our factor base, by the prime number theorem we expect that $p_j \simeq 2j \log j$, and so $\alpha_j \simeq c/j$.

We now let A be an $l \times k$ binary array, entries chosen independently, in which the probability that an entry in column j is 1 is $\alpha_j = c/j$. We now consider the number of empty columns, the number of columns with exactly one 1 (which we will refer to as a *solon* for solo 1), and the number of columns containing exactly two 1's (which we will refer to as *colons*). Let $X_r(A)$ be the number of columns containing exactly r 1's. Earlier we considered the number of nonempty columns, $k - X_0$. We now refine our analysis to include solons. We will take colons into account later.

If a column is a solon, then the row containing the corresponding 1 cannot appear in a nontrivial row-dependency. Thus, we can replace A by the array with the solon and its corresponding row removed. Since two solons can have the same row containing their solo 1, we can remove more columns than rows. There are $X_1(A)$ solons, and for each solon every row is equally likely to contain the solo 1. Hence, the probability that a given row is not deleted is

$$\left(1 - \frac{1}{l}\right)^{X_1} \simeq e^{-X_1/l},$$

and so the expected number of rows left after deleting X_1 solons is about $le^{-X_1/l}$. Now the rows of array A are linearly dependent if

$$e^{-X_1/l} l > k - X_0 - X_1.$$

Computing expected values here,

$$E(X_0) \simeq \sum_{j=1}^{k} e^{-l\alpha_j} \simeq \int_1^k e^{-cl/x}\, \mathrm{d}x$$
$$\simeq \int_0^k e^{-cl/x}\, \mathrm{d}x = ke^{-cl/k} - clEi(1, cl/k)$$

in which $Ei(a,b) = \int_1^\infty e^{-bx}x^{-a}\,\mathrm{d}x$ is the exponential integral (as defined by *Maple*). Furthermore,

$$\begin{aligned} E(X_1) &\simeq \sum_{j=1}^{k} l\alpha_j e^{-l\alpha_j} \simeq \int_1^k \frac{cl}{x} e^{-cl/x}\,\mathrm{d}x \\ &\simeq \int_0^k \frac{cl}{x} e^{-cl/x}\,\mathrm{d}x = clEi(1, cl/k). \end{aligned}$$

So we expect that the number of rows and columns remaining will be equal after removing empty columns and solons if

$$l\exp(-E(X_1)/l) = k - E(X_0) - E(X_1)$$

is satisfied; that is,

$$l\exp(-cEi(1, cl/k)) = k(1 - \exp(-cl/k)).$$

Solving this equation numerically with *Maple*, we obtain the following values:

c	l/k threshold
0.2	0.0008980931
0.4	0.1400018494
0.6	0.4119714260
0.8	0.6120819888
1.0	0.7394711744
1.2	0.8207464220
1.4	0.8739519006
1.6	0.9097291738
1.8	0.9343624832
2.0	0.9516659561

For the value $c = 0.72$ (which arises in the experimental evidence discussed below), we obtain a threshold of .5423300259.

6.6.2 Reducing the Size of the Final Linear Algebra Problem

We now include colons in our analysis: Their impact is not to reduce the number of rows needed to obtain the first dependency (there is a small impact, but it is negligible, so we won't discuss it), but rather to reduce the size of the final linear algebra question under consideration.

Suppose that a column is a colon, that is, it contains exactly two 1's, and that these 1's appear in rows r_1 and r_2. Then, in any linear combination of rows summing to zero, either both the rows r_1 and r_2 appear, or neither appear. Hence, the rows of A are linearly dependent if and only if the rows of A' are, where A' is the array obtained by replacing r_1 by $r_1 + r_2$, replacing r_2 by $\underline{0}$, and deleting the colon-column.

A good combinatorial model for this is to take a graph G having as vertex set the set of rows of A and as edge set the set of pairs $\{r_1, r_2\}$ corresponding to colons. Then, replacing rows by their sum corresponds to contracting edges in the graph, replacing connected components by a single vertex. Components containing a vertex corresponding to a 1 appearing in a solon get deleted completely.

This enables us to reduce the size of the array A considerably: If we have no cycles in the graph, then the contraction of each edge reduces the number of components by 1. Furthermore, when we contract edges or delete components in the graph, we can create new edges (for example, if a column in A contains four 1's, in rows r_1, r_2, r_3, and r_4, and if we have a colon with 1's in rows r_1 and r_2, then when we replace r_1 with $r_1 + r_2$ and r_2 with $\underline{0}$, the four 1's will become a colon).

6.7 Experimental Evidence

The students involved in this project ran several different experiments, and we have followed up on these. To begin with, Tim Flowers implemented the quadratic sieve to produce real data. Working with n around 10^{15} and a factor base bound $B = \exp(\sqrt{\log(n)\log\log(n)})$, iterated deletions reduced arrays of size around 500×2000 to arrays of size around 65×60.

In addition, the arrays produced suggest that (for n in this range) the probabilities α_j satisfy $\alpha_j \simeq 0.72/j$.

We fixed $c = 0.72$ and constructed random arrays of size $l \times k$, for various values of l, k, and computed various statistics:

- the proportion of successful trials, trials for which iterated removal of solons and colons left an array with more nonzero rows than columns (implying the rows of the initial array are linearly dependent);

- the proportion of trials for which iterated removal of solons and colons left a nonzero array with at most as many rows as columns (so that we can't conclude that the rows of the initial array are linearly dependent);

- the maximum and minimum number of nonzero rows and columns remaining after iterated removal of solons and colons;

- the average number of rows and columns remaining after iterated removal of solons and colons.

We observed in almost all trials that we either ended up with a zero matrix (so the original rows were independent) or with more rows than columns (so the original rows were dependent). This is consistent with the following conjecture:

Conjecture 6.3. *Generate vectors in GF_2^k independently with $\alpha_j = 0.72/j$. Then almost surely (in the sense that the probability approaches 1 as $k \to \infty$) the first linear dependency gives a matrix that reduces to a $t+1 \times t$ matrix after iterated removal of solons and colons.*

Essentially, this conjecture says that there are two conditions, one of which implies the other, and that usually, the two coincide exactly. This is a common situation in the theory of random graphs, in which, for example, if the edges of the complete graph on n vertices are placed in random order, the edge that makes the graph connected is almost surely the edge that makes the minimum degree equal to 1.

In studying threshold functions for the occurrence of combinatorial structures, for example in random graphs (see, for example, Bollobas [39]), it is frequently the case that the threshold behaves (suitably scaled) like the function $e^{-e^{-x}}$. Figure 6.1 shows the proportion of successful trials with $k = 20{,}000$, for l from 1000, 1100, 1200, ... 3000, with 100 trials each. Figure 6.2 shows the function $e^{-e^{-x}}$, suitably scaled and shifted to match this. The overlay of the two pictures in Figure 6.3 shows that the match is close but not perfect. However, it is close enough to suggest that there is a similar threshold behavior going on.

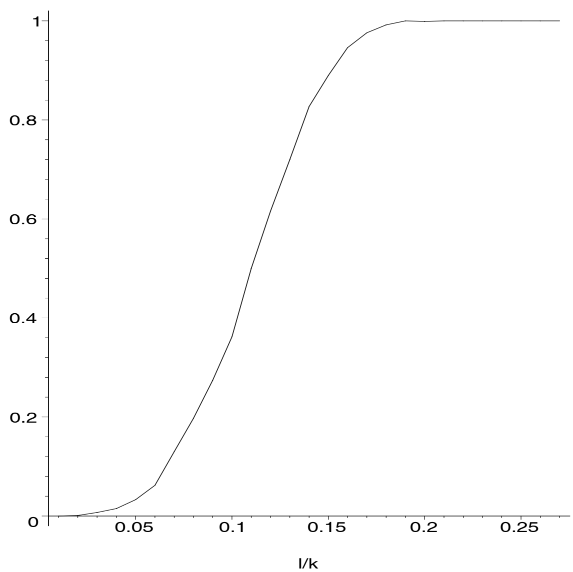


Figure 6.1. Probability l rows of length 20,000 are dependent.

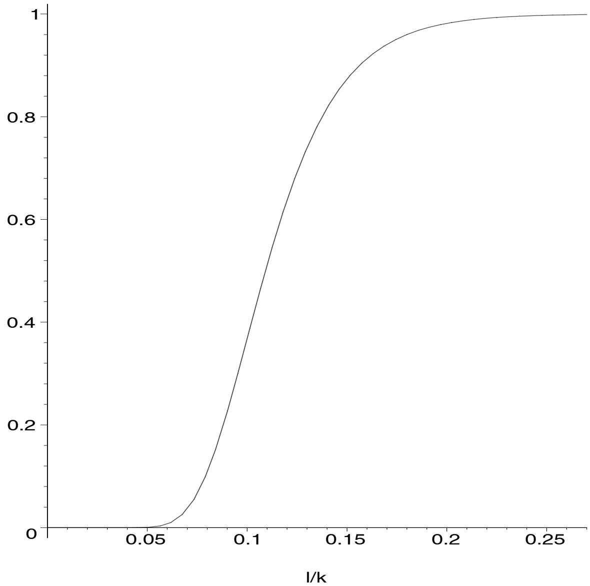


Figure 6.2. Scaled, shifted plot of $e^{-e^{-x}}$.

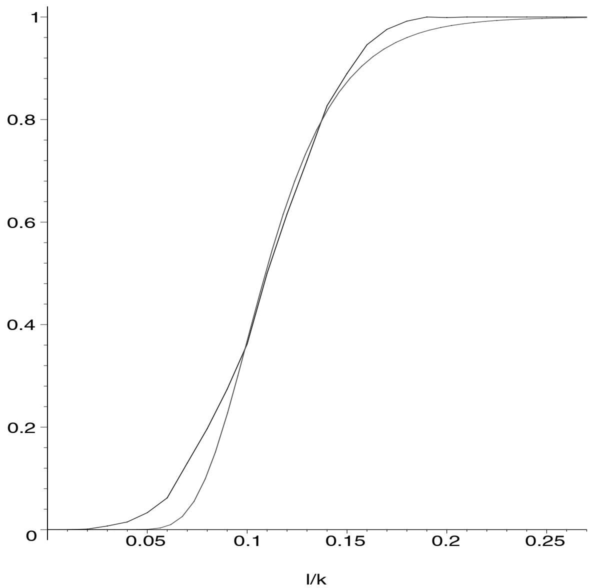


Figure 6.3. Overlay of probability, $e^{-e^{-x}}$.

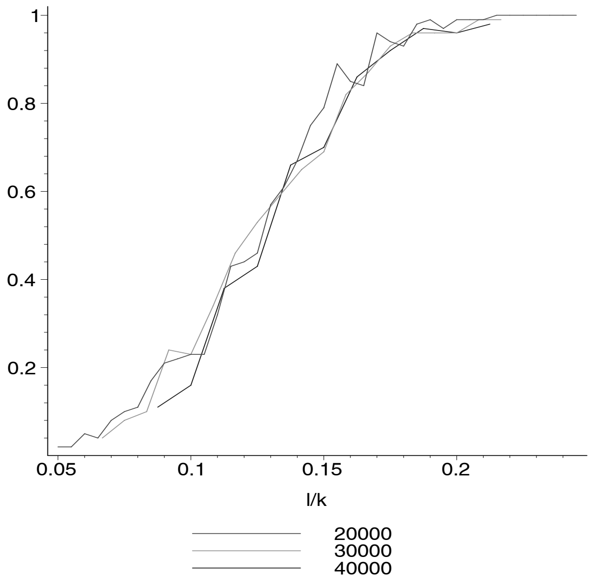


Figure 6.4. Probabilities of dependencies for various l, $k = 20{,}000, 30{,}000, 40{,}000$.

We can also compare the threshold functions for finding dependence this way for various values of k. Figure 6.4 shows the proportion of successes for $k =$ 20,000, 30,000 and 40,000: The horizontal axis is scaled to give l/k. This figure is consistent with the hypothesis that there is a sharp threshold β around 0.2.

6.8 Conclusions

After considering various probabilistic possible models for the Quadratic Sieve, it appears that we have found one which is a reasonably good match. Since almost all of our arguments were heuristic and our evidence almost purely experimental, there are two obvious routes to follow now. First, implement the Quadratic Sieve to take account of the ideas discussed here, and estimate the improved runtime. Second, put the heuristics on a sounder footing, proving some of the natural assumptions that we have made. We are currently working on both of these tasks.

One of the advantages of removing solons and colons is that it can be done in parallel: Most linear algebra algorithms are rather hard to parallelize, so if we can preprocess the matrix in this fashion, then it may make the remaining linear algebra tasks much faster to perform. (In addition, if the iterated deletions can be parallelized effectively, it is *possible* that this might make the Quadratic

Sieve faster in implementations than algorithms such as the Number Field Sieve in which the linear algebra phase is hard to parallelize.)

One might ask why these techniques have not been used already. It appears to be the case that they only become useful if l is sufficiently *small* compared to k, and since most implementations aimed to get l *large* in order to ensure dependency, the usefulness of iterated deletion of solons and colons has not been noticed.

While it is clear that the ideas here will speed up the Quadratic Sieve, we don't expect that this will have a huge impact: Currently the Quadratic Sieve is only the second fastest general purpose factoring algorithm, and the improvements suggested here are unlikely to lift it into first place. The fastest algorithm, the General Number Field Sieve, is similar in nature, in that it generates a sequence of vectors over GF_2 and a linear dependency is used to generate a factorization. However, heuristics suggest that the vectors generated are somewhat denser than for the Quadratic Sieve, perhaps having $\alpha_j = c \log j / j$. If this is the case, then the expected number of solons and colons is so small that the techniques discussed here will not have any effect.

7 A Selection of Integrals from a Popular Table

> I see some parallels between the shifts of fashion in mathematics and in music. In music, the popular new styles of jazz and rock became fashionable a little earlier than the new mathematical styles of chaos and complexity theory. Jazz and rock were long despised by classical musicians, but have emerged as art-forms more accessible than classical music to a wide section of the public. Jazz and rock are no longer to be despised as passing fads. Neither are chaos and complexity theory. But still, classical music and classical mathematics are not dead. Mozart lives, and so does Euler. When the wheel of fashion turns once more, quantum mechanics and hard analysis will once again be in style.
>
> —Freeman Dyson[1]

7.1 The Allure of the Integral

The evaluation of definite integrals is one of the most intriguing topics of elementary mathematics. Every student of Calculus is exposed to a variety of techniques that *sometimes* work, but they always leave the feeling of just being a collection of tricks.

The goal of this chapter is to introduce the reader to the methods of experimental mathematics in the context of definite integrals. We hope to convey that, in spite of wonderful collections such as *Tables of Integrals, Series and Products* by I. S. Gradshteyn and I. M. Rhyzik [149] and sophisticated symbolic languages such as *Mathematica*, there is a lot of interesting things to do. The use of *Mathematica* is essential in our approach to this question.

One of the features of definite integration is that similar integrands produce problems of different levels of complexity. The reader is already aware of this phenomenon: The integral

$$\int_0^\infty e^{-x}\,dx = 1 \tag{7.1}$$

is elementary; the normal integral

$$\int_0^\infty e^{-x^2}\,dx = \frac{\sqrt{\pi}}{2} \tag{7.2}$$

[1] In his review of *Nature's Numbers* by Ian Stewart (Basic Books, 1995), on p. 612 of *American Mathematical Monthly*, August–September 1996.

can be obtained by elementary methods, but the next example in this family,

$$\int_0^\infty e^{-x^3}\,dx = \Gamma\left(\frac{4}{3}\right), \tag{7.3}$$

requires the introduction of the *Gamma function*

$$\Gamma(x) := \int_0^\infty t^{x-1}e^{-t}\,dt \tag{7.4}$$

to obtain the answer. This is the remarkable function that satisfies

$$\Gamma(n+1) = n!, \tag{7.5}$$

so it provides an analytic extension of factorials. Under some mild conditions this is in fact unique. Note also the *duplication formula*

$$\Gamma(2x) = 2^{2x-1}\Gamma\left(x+\tfrac{1}{2}\right)\Gamma(x)/\Gamma\left(\tfrac{1}{2}\right) \tag{7.6}$$

and the *reflection formula*

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}. \tag{7.7}$$

The evaluation (7.2) corresponds to the special value

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}, \tag{7.8}$$

following from the reflection formula for $z = 1$. At this point it is natural to ask whether $\Gamma(4/3)$ in (7.3) can be expressed in terms of more elementary functions. This is a difficult question that will not be addressed here, but see [90] for an introduction.

The fact that definite integrals are given as specific values of special functions is familiar to students. This is central to the question of what constitutes an *acceptable answer* to a required evaluation. For instance, every student will evaluate

$$\int_0^1 \frac{dx}{\sqrt{2-x^2}} = \frac{\pi}{4} \tag{7.9}$$

and consider it a reasonably good answer, but the similar problem

$$\int_0^1 \frac{dx}{\sqrt{9-x^2}} = \arcsin\left(\frac{1}{3}\right) \tag{7.10}$$

will force the issue of *simplifying the answer*. Even at this level, this is related to deep, interesting questions: For which integers n is the number $\sin(\pi/n)$ expressable in radicals? It is surprising to the beginner that the answer lies in the realm of abstract algebra. See [264] for a historical discussion of this topic.

A remarkable feature of integration is that *complicated real numbers* appear as definite integrals, in which the integrand is relatively simple. One does not need to complicate the integrand to produce a difficult problem. For example, in entry 4.241.11 of [149] we find

$$\int_0^1 \frac{\log x \, dx}{\sqrt{x(1-x^2)}} = -\frac{\sqrt{2\pi}}{8}\left[\Gamma\left(\frac{1}{4}\right)\right]^2. \tag{7.11}$$

The Gamma function defined in (7.4) makes a new appearance. The concept of *complicated* needs to be formalized, but it should be clear that (7.11) is more complicated than (7.10).

The reader will find in [44] many other interesting features involved in the evaluation of definite integrals.

7.2 The Project and Its Experimental Nature

The central question of our research can be described in simple terms: Given a function

$$f = f(x; p_1, p_2, \cdots, p_n) \tag{7.12}$$

that depends on a set of *parameters*: $p_1, \cdots, p_n$, we want to express the definite integral

$$I = I(f; p_1, \cdots, p_n; a, b) = \int_a^b f(x; p_1, p_2, \cdots, p_n)\, dx \tag{7.13}$$

in terms of the parameter set $\{p_1, \cdots, p_n, a, b\}$.

As such, the problem is too general and simple to solve. Define g to be a *primitive* of f and use the fundamental theorem of calculus to evaluate I. The problem becomes more interesting if we fix the class of possible primitives. For instance, given a *rational function* f, find the value of I in the rational class.

Our long term plan is to develop a *complete theory of definite integration*. As a special part of this project, we would like to provide proofs of the many formulas appearing in the classical table of integrals, such as [149]. The material presented there is enormous. This collection has as ancestors the table compiled by Bierens de Haan [37] and the beautifully typed tables [152] and [153]. There are some new tables that present interesting evaluations, for instance A. Apelblat [6].

In these notes we present some of the methods that we use in our work. Two aspects that appear throughout this presentation are

1. *Integral representations.* Many special functions admit representations as integrals. For example,

$$\arctan x = \int_0^x \frac{dt}{1+t^2}. \tag{7.14}$$

We read these representations from right to left, that is, we see the special function as giving us evaluations of the definite integral.

2. *Interesting numbers.* The values of integrals produce real numbers that appear in other contexts. For example,

$$\int_0^\infty \frac{t^{x-1}\,dt}{e^t+1} = (1-2^{1-x})\Gamma(x)\zeta(x), \tag{7.15}$$

where

$$\zeta(x) = \sum_{n=1}^\infty \frac{1}{n^x} \tag{7.16}$$

is, again, the famous Riemann zeta function. This function appeared in the study of distribution of prime numbers, and its zeroes are worth some money.[2] See [92], especially the article by Peter Sarnak on that website. Therefore, its special values have some intrinsic interest. We think of special values of interesting functions as the *primitive blocks* that form real numbers. For instance,

$$\int_0^{\pi/2} \left(\frac{x}{\sin x}\right)^4 dx = -\frac{1}{12}\pi^3 + 2\pi\log 2 + \frac{1}{3}\pi^3\log 2 - \frac{3}{2}\pi\zeta(3) \tag{7.17}$$

is an expression formed by the blocks $\log 2, \pi$, and $\zeta(3)$. The problem of simplification of these combinations is rather difficult: If the expression $\zeta(4)/\pi^4$ appears, then it has been known since Euler that it reduces to $1/90$. On the other hand, we do not know much about $\zeta(3)/\pi^3$; the case of odd values of ζ seems to be much more difficult. As W. Zudilin phrases it, "A general feeling is that π, $\zeta(3)$, $\zeta(5)$, $\zeta(7), \ldots$ are algebraically independent, but this seems to be a problem forever."

7.3 Families and Individuals

Among the formulas presented in [149], some of them can be treated as members of a larger family. For example, in entry 4.224.6 we find

$$\int_0^{\pi/2} \log\cos x\,dx = -\frac{\pi}{2}\log 2 \tag{7.18}$$

that is related to entry 4.224.8:

$$\int_0^{\pi/2} (\log\cos x)^2\,dx = \frac{\pi}{2}\left[(\log 2)^2 + \frac{\pi^2}{12}\right]. \tag{7.19}$$

[2] We believe that there are much easier ways to make $1,000,000.

This leads to the consideration of the general case

$$LC_n := \int_0^{\pi/2} (\log\cos x)^n \, dx. \tag{7.20}$$

A direct symbolic computation yields

$$\begin{aligned} LC_1 &= -\tfrac{1}{2}ac, \\ LC_2 &= \tfrac{1}{2}a^2c + \tfrac{1}{24}c^3, \\ LC_3 &= -\left(\tfrac{1}{2}a^3c + \tfrac{3}{4}b^3c + \tfrac{1}{8}ac^3\right), \\ LC_4 &= \tfrac{1}{2}a^4c + 3ab^3c + \tfrac{1}{4}a^2c^3 + + \tfrac{19}{480}c^5, \end{aligned} \tag{7.21}$$

where we have employed the notation $a := \log 2$, $b := \zeta(3)^{1/3}$, $c := \pi$.

While the values of $\zeta(2n)$ have been well known since the eighteenth century to be rational multiples of π^{2n}, see (3.17), the situation for the odd values of ζ is much more difficult. The reader can find in [271] an informal report on the reaction to the proof of irrationality of $\zeta(3)$ given by R. Apéry. The constant $\zeta(3)$ has become known as *Apéry's constant*. A different proof of this result was presented by F. Beukers in [35]. His proof is based on the representation

$$\int_0^1 \int_0^1 \frac{P_n(x)P_n(y)}{1-xy} \log xy \, dx \, dy = 2(a_n - b_n\zeta(3)). \tag{7.22}$$

Here b_n are integers, a_n are rationals numbers such that $2\text{LCM}[1,\cdots,n]a_n$ is an integer, and

$$P_n(z) = \frac{1}{n!}\frac{d^n}{dz^n}\left[z^n(1-z)^n\right] \tag{7.23}$$

is the classical Legendre polynomial. This is one more instance of integrals at the center of interesting mathematics.

From the data in (7.21) we see that $(-1)^n LC_n$ is a polynomial in the variables a, b, c with positive rational coefficients. Morever, this is a homogeneous polynomial of degree $n+1$. Using a symbolic language we can test this conjecture. Indeed, the next term in the family is

$$LC_5 = -\left(\frac{1}{2}a^5c + \frac{15}{2}a^2b^3c + \frac{5}{12}a^3c^3 + \frac{5}{8}b^3c^3 + \frac{19}{96}ac^5 + \frac{45}{4}cd^5\right), \tag{7.24}$$

where the new variable d is $\zeta(5)^{1/5}$. The conjecture has now been verified for $n = 5$.

The next steps in the analysis of this example are

- prove the conjecture (the reader will find in [36] a recurrence for the integrals LC_n—this should help);

- discover a reason for its existence;
- find a closed form for the coefficients in LC_n.

There are some other evaluations that seem to be *individuals*. The formula 4.229.7

$$\int_{\pi/4}^{\pi/2} \log\log\tan x\, dx = \frac{\pi}{2}\log\left\{\frac{\Gamma(3/4)}{\Gamma(1/4)}\sqrt{2\pi}\right\}, \tag{7.25}$$

which is the subject of the delightful paper by Ilan Vardi [272], is apparently in this category. The proof of (7.25) is based on Dirichlet L-series. This is evidence that to evaluate integrals one needs to learn analytic number theory.

The flexibility provided by changes of variables permits us to represent Vardi's integrals in many forms. Some of these can be found in [149]. The new variable $u = \log\tan x$ gives entry 4.371.1:

$$\int_0^\infty \frac{\log u}{\cosh u}\, du = \pi\log\left\{\frac{\Gamma(3/4)}{\Gamma(1/4)}\sqrt{2\pi}\right\}. \tag{7.26}$$

One of the advantages of a table in paper form is that it allows for browsing. A neighbor of the previous integral is entry 4.371.3,

$$\int_0^\infty \frac{\log x\, dx}{\cosh^2 x} = \log\pi - 2\log 2 - \gamma, \tag{7.27}$$

where γ is again the Euler-Mascheroni constant. The question of whether γ is rational is still open. We are sure that definite integrals will appear in its solution. J. Sondow has many interesting examples of integrals for γ [258].

The two examples mentioned above are part of the family

$$LT_n := \int_0^\infty \frac{\log x\, dx}{\cosh^n x}. \tag{7.28}$$

We encourage the reader to use a symbolic language to explore this new series of integrals.

Browsing also allows us to find interesting examples in [149]. For instance, on page 575 we find entry 4.375.1 as

$$\int_0^\infty \log\cosh\frac{x}{2}\,\frac{dx}{\cosh x} = G + \frac{\pi}{4}\log 2 \tag{7.29}$$

and a symbolic evaluation reveals that there is a sign error: The correct value of the integral is $G - \frac{\pi}{4}\log 2$. Here G is Catalan's constant, as in Chapter 2. The value of this integral appears written correctly as formula BI(259)(11) in [37]. It appears there in the equivalent form

$$\int_0^\infty \frac{\log(e^{x/2}+e^{-x/2})}{e^x+e^{-x}}\, dx = \frac{\pi}{8}\log 2 + \frac{1}{2}\sum_{n=0}^\infty \frac{(-1)^n}{(2n+1)^2}. \tag{7.30}$$

Symbolic extensions of this example are not very successful: My current version of *Mathematica* is unable to evaluate

$$\int_0^\infty \log\cosh\frac{x}{3}\,\frac{dx}{\cosh x}. \tag{7.31}$$

One of the intrinsic problems with symbolic languages is that the result in the evaluation depends on how the integrand is input. For instance, *Mathematica* gives the value of

$$\begin{aligned}
&\int_0^\infty \log\cosh x\,\frac{dx}{\cosh 3x}\\
&= \frac{1}{18}\Bigg[16G - 3\pi\log\left(\frac{4}{3}\right) + 6i\left(\mathrm{Li}_2\left(\left(\frac{1}{6}+\frac{i}{6}\right)\left(3-i\sqrt{3}\right)\right)\right.\\
&\quad +\mathrm{Li}_2\left(-\frac{1+i}{-i+\sqrt{3}}\right) - \mathrm{Li}_2\left(\frac{1-i}{-i+\sqrt{3}}\right) - \mathrm{Li}_2\left(-\frac{1-i}{i+\sqrt{3}}\right)\\
&\quad +\mathrm{Li}_2\left(\frac{1+i}{i+\sqrt{3}}\right) - \mathrm{Li}_2\left(\left(\frac{1}{6}+\frac{i}{6}\right)\left(-3i+\sqrt{3}\right)\right)\\
&\quad \left.+\mathrm{Li}_2\left(-\frac{2-2i}{3i+\sqrt{3}}\right) - \mathrm{Li}_2\left(\left(-\frac{1}{6}-\frac{i}{6}\right)\left(3i+\sqrt{3}\right)\right)\right)\Bigg],
\end{aligned} \tag{7.32}$$

where G is Catalan's constant and Li is the polylogarithm function defined in (2.12). Judging by the symmetry of the polylogarithm arguments in this integral evaluation, it seems likely that this can be written in terms of Clausen function evaluations (see (9.101) below).

7.4 An Experimental Derivation of Wallis' Formula

The evaluation

$$J_{2,m} := \int_0^\infty \frac{dx}{(x^2+1)^{m+1}} = \frac{\pi}{2^{2m+1}}\binom{2m}{m} \tag{7.33}$$

is presented in some calculus books. We present here an experimental derivation of it.

The first step is to produce convincing evidence that the right-hand side of (7.33) is correct. This can be achieved by a symbolic evaluation of the integral. The *Mathematica* command

```
Integrate[1/(x^2+1)^(m+1), {x,0,Infinity}]
```

requests the value of $J_{2,m}$. The response involves the condition $\mathrm{Re}\,m > -\frac{1}{2}$ that guarantees convergence of the integral. This can be added to the request via the command

```
Assumptions -> Re[m] > -1/2.
```

The answer provided by *Mathematica* is given in terms of the Gamma function as

$$J_{2,m} = \frac{\sqrt{\pi}}{2} \frac{\Gamma(\frac{1}{2}+m)}{\Gamma(1+m)}. \tag{7.34}$$

The expression for $J_{2,m}$ given in (7.33) now follows directly from the duplication formula for the Gamma function (7.6) and the value $\Gamma(n) = (n-1)!$ for $n \in \mathbb{N}$.

We now present an alternative process for obtaining (7.33) as an example of our experimental technique. Using a symbolic language such as *Mathematica*, we obtain the first few values of $J_{2,m}$ as

$$\left\{ \frac{\pi}{4}, \frac{3\pi}{16}, \frac{5\pi}{32}, \frac{35\pi}{256}, \frac{63\pi}{512}, \frac{231\pi}{2048} \right\}. \tag{7.35}$$

It is reasonable to conjecture $J_{2,m}$ as a rational multiple of π. We now begin the exploration of this rational number by defining the function

$$f_2(m) := \text{Denominator}(J_{2,m}/\pi). \tag{7.36}$$

Use the command

```
FactorInteger[Denominator[J[2,m]/Pi]]
```

to conclude that the denominator of $f_2(m)$ is a power of 2. Making a list of the first few exponents, we (experimentally) conclude that

$$f_3(m) := 2^{2m} f_1(m)/\pi \tag{7.37}$$

is an integer. The first few values of this function are

$$\{1, 3, 10, 35, 126, 462, 1716, 6435, 24310, 92378\}. \tag{7.38}$$

Now comes the difficult part: We want to obtain a closed form expression for $f_3(m)$ directly from this list. For this we employ the *Online Encyclopedia of Integer Sequences* at the site [255] http://www.research.att.com/~njas/sequences/. Entering the first four values we find that

$$f_3(m) = \binom{2m+1}{m+1} \tag{7.39}$$

is reasonable. This can be checked by computing more data. The expression for f_3 leads to the proposed form of $J_{2,m}$.

The exploration of Sloane's list is also a wonderful learning experience. The reader should use it and learn about the sequence

$$\{1, 3, 10, 35, 126, 462, 1717\} \tag{7.40}$$

that we got when we made a mistake and typed 1717 instead of 1716.

We now prove that

$$J_{2,m} = \int_0^\infty \frac{dx}{(x^2+1)^{m+1}} = \frac{\pi}{2^{2m+1}}\binom{2m}{m}, \tag{7.41}$$

where m is a nonnegative integer. The change of variables $x = \tan\theta$ converts $J_{2,m}$ to its trigonometric form

$$J_{2,m} = \int_0^{\pi/2} \cos^{2m}\theta\, d\theta = \frac{\pi}{2^{2m+1}}\binom{2m}{m}, \tag{7.42}$$

which is known as Wallis's formula. The proof of (7.42) is elementary and sometimes found in calculus books (see, e.g., [192, p. 492].). It consists of first writing $\cos^2\theta = 1 - \sin^2\theta$ and using integration by parts to obtain the recursion

$$J_{2,m} = \frac{2m-1}{2m} J_{2,m-1}, \tag{7.43}$$

and then verifying that the right-hand side of (7.42) satisfies the same recursion and that both sides yield $\pi/2$ for $m = 0$.

We now present a new proof of Wallis's formula. We have

$$J_{2,m} = \int_0^{\pi/2} \cos^{2m}\theta\, d\theta = \int_0^{\pi/2} \left(\frac{1+\cos 2\theta}{2}\right)^m d\theta.$$

Now introduce $\psi = 2\theta$ and expand and simplify the result by observing that the odd powers of cosine integrate to zero. The inductive proof of (7.42) requires

$$J_{2,m} = 2^{-m} \sum_{i=0}^{[m/2]} \binom{m}{2i} J_{2,i}. \tag{7.44}$$

Note that $J_{2,m}$ is uniquely determined by (7.44) along with the initial value $J_{2,0} = \pi/2$. Thus, (7.42) now follows from the identity

$$f(m) := \sum_{i=0}^{[m/2]} 2^{-2i} \binom{m}{2i}\binom{2i}{i} = 2^{-m}\binom{2m}{m} \tag{7.45}$$

since (7.45) can be written as

$$A_m = 2^{-m} \sum_{i=0}^{[m/2]} \binom{m}{2i} A_i,$$

where

$$A_i = \frac{\pi}{2^{2i+1}}\binom{2i}{i}.$$

It remains to verify the identity (7.45). This can be done *mechanically* using the theory developed by Wilf and Zeilberger, which is explained in [220,229]; the sum in (7.45) is the example used in [229] (page 113) to illustrate their method. The *Maple* command

```
ct(binomial(m,2i)  binomial(2i,i) 2^{-2i},
1, i, m, N)
```

produces

$$f(m+1) = \frac{2m+1}{m+1} f(m), \tag{7.46}$$

and one can check that $2^{-m}\binom{2m}{m}$ satisfies the same recursion. Note that (7.43) and (7.46) are equivalent since

$$J_{2,m} = \frac{\pi}{2^{m+1}} f(m).$$

This proof is more complicated than using (7.43), but the method behind it applies to other rational integrals. This was the first step in a series of results on rational Landen transformations. The reader will find in [43] the details for even rational functions and should see [207] for recent developments.

7.5 A Hyperbolic Example

Section 3.511 of the table of integrals [149] contains the evaluation of several definite integrals whose integrands are quotients of hyperbolic functions. For instance, entry 3.511.2 reads

$$\int_0^\infty \frac{\sinh(ax)}{\sinh(bx)}\,dx = \frac{\pi}{2b}\tan\frac{a\pi}{2b} \tag{7.47}$$

while the next formula 3.511.3 is

$$\int_0^\infty \frac{\sinh(ax)}{\cosh(bx)}\,dx = \frac{\pi}{2b}\sec\frac{a\pi}{2b} - \frac{1}{b}\beta\left(\frac{a+b}{2b}\right). \tag{7.48}$$

(As usual, we use the secant $\sec = 1/\cos$ and the cosecant $\csc = 1/\sin$.) The reader will find in [149], formula 8.371.1, the function β given by the integral representation

$$\beta(x) = \int_0^1 \frac{t^{x-1}}{1+t}\,dt. \tag{7.49}$$

We introduce the notation

$$g_1(a,b) = \int_0^\infty \frac{\sinh(ax)}{\cosh(bx)}\,dx \tag{7.50}$$

and now discuss its evaluation. Naturally the answer given in the table is in terms of the β-function, so its integral representation suggests a procedure for how to start. *Checking the value of an integral is much easier than finding it.* Simply let $t = e^{-2bx}$ to obtain

$$g_1(a,b) = \frac{1}{2b}\beta\left(\frac{1}{2} - \frac{a}{2b}\right) - \frac{1}{2b}\beta\left(\frac{1}{2} + \frac{a}{2b}\right). \tag{7.51}$$

We now use properties of β to reduce this answer to the one given in [149]. This function is related to the classical *digamma* or *psi* function

$$\psi(x) := \frac{\Gamma'(x)}{\Gamma(x)} \tag{7.52}$$

via

$$\beta(x) = \frac{1}{2}\left(\psi\left(\frac{x+1}{2}\right) - \psi\left(\frac{x}{2}\right)\right). \tag{7.53}$$

The functional equation for the Gamma function

$$\Gamma(1+x) = x\Gamma(x) \tag{7.54}$$

yields the identity

$$\psi(1+x) = \psi(x) + \frac{1}{x}. \tag{7.55}$$

In turn this produces

$$\beta(x+1) = -\beta(x) + \frac{1}{x}. \tag{7.56}$$

Similarly,

$$\psi(1-x) = \psi(x) + \pi\cot\pi x \tag{7.57}$$

produces

$$\beta(1-x) = -\beta(x) + \pi\csc\pi x. \tag{7.58}$$

Using these identities in (7.51) yields (7.48).

But suppose that the reader is not familiar with these functions. Is there anything that one can learn from the integrals by using a symbolic language?

A blind evaluation[3] produces an answer in terms of the function

$$h(x) := \text{HarmonicNumber}[x] := \sum_{k=1}^{\infty}\left(\frac{1}{k} - \frac{1}{k+x}\right) \tag{7.59}$$

[3] This is one in which we simply input the question and ask *Mathematica* for an answer.

as

$$\begin{aligned} g_1(a,b) &= \frac{\text{HarmonicNumber}\left[\frac{1}{4}(-3+\frac{a}{b})\right]}{4b} \\ &-\frac{\text{HarmonicNumber}\left[\frac{1}{4}(-1+\frac{a}{b})\right]}{4b} \\ &+\frac{\text{HarmonicNumber}\left[-\frac{a+b}{4b}\right]}{4b} \\ &-\frac{\text{HarmonicNumber}\left[-\frac{a+3b}{4b}\right]}{4b}. \end{aligned}$$

The answer is written here exactly as it appears in the *Mathematica* code. To simplify it, we apply the command

```
FunctionExpand
```

which produces

$$\begin{aligned} g_1(a,b) &= -\frac{\text{PolyGamma}\left[0,\frac{1}{4}-\frac{a}{4b}\right]}{4b}+\frac{\text{PolyGamma}\left[0,\frac{3}{4}-\frac{a}{4b}\right]}{4b} \\ &+\frac{\text{PolyGamma}\left[0,\frac{1}{4}+\frac{a}{4b}\right]}{4b}-\frac{\text{PolyGamma}\left[0,\frac{3}{4}+\frac{a}{4b}\right]}{4b}. \end{aligned}$$

The polygamma function appearing here is simply $\psi(x)$, and it is easy to see that this expression for g_1 is equivalent to (7.51). We also see from here that $4bg_1(a,b)$ is a function of the single parameter $c=\frac{a}{b}$. This is elementary. The change of variables $t=bx$ yields

$$4bg_1(a,b)=4\int_0^\infty \frac{\sinh(ct)}{\cosh t}\,dt. \tag{7.60}$$

Thus, we write

$$g_2(c)=4bg_1(a,b), \tag{7.61}$$

and the previous evaluation is written as

$$\begin{aligned} g_2(c) &= -\text{PolyGamma}\left[0,\tfrac{1}{4}-\tfrac{c}{4}\right]+\text{PolyGamma}\left[0,\tfrac{3}{4}-\tfrac{c}{4}\right] \\ &+\text{PolyGamma}\left[0,\tfrac{1}{4}+\tfrac{c}{4}\right]-\text{PolyGamma}\left[0,\tfrac{3}{4}+\tfrac{c}{4}\right]. \end{aligned}$$

In order to obtain some information about the function g_2, we can use *Mathematica* to create a list the values $g_2(n)$ for $n=1,\ldots,10$. Note that, for these values, the integral (7.48) itself is not convergent. Instead, we are interested here in the analytic continuation. The command

```
T_{1} :=  Table[g_{2}[n], {n,1, 10}]
```

then produces

$$T_1 = \left\{\infty, -8, \infty, \tfrac{16}{3}, \infty, -\tfrac{104}{15}, \infty, \tfrac{608}{105}, \infty, -\tfrac{2104}{315}\right\}. \tag{7.62}$$

This indicates the presence of singularities for the function g_2 at the odd integers and a clear pattern for the signs at the even ones. We then compute the table of values of $(-1)^n g_2(2n)$ for $1 \leq n \leq 9$:

$$T_2 = \left\{8, \tfrac{16}{3}, \tfrac{104}{15}, \tfrac{608}{105}, \tfrac{2104}{315}, \tfrac{20624}{3465}, \tfrac{295832}{45045}, \tfrac{271808}{45045}, \tfrac{4981096}{765765}\right\}.$$

From here we experimentally conclude that g_2 has a singularity at the odd integers and that $r_n = (-1)^n g_2(2n)$ is a positive rational number. We leave the singularity question aside and explore the properties of the sequence r_n.

The beginning of the sequence of denominators agrees with that of the *odd semi-factorials*:

$$(2n-1)!! := (2n-1)\cdot(2n-3)\cdot(2n-5)\cdots 5\cdot 3\cdot 1 \tag{7.63}$$

that begins as

$$T_3 = \{1, 3, 15, 105, 945, 10395, 135135, 2027025\}. \tag{7.64}$$

Thus, it is natural to consider the function

$$g_3(n) = (-1)^n(2n-1)!!g_2(2n). \tag{7.65}$$

The hope is that $g_3(n)$ is an integer valued function. The first few values are given by

$$T_4 = \{8, 16, 104, 608, 6312, 61872, 887496, 12231360\}. \tag{7.66}$$

Observe that they are all even integers. To examine their divisibility in more detail, we introduce the concept of p-adic valuation.

Let $n \in \mathbb{N}$ and p be a prime. The p-adic valuation of n, denoted by $\nu_p(n)$, is defined as the exact power of p that divides n. Now define

$$g_4(n) = \nu_2(g_3(n)), \tag{7.67}$$

and its first few values are

$$T_5 = 3 + \{0, 1, 0, 2, 0, 1, 0, 3, 0, 1, 0, 2, 0, 1, 0, 4\}, \tag{7.68}$$

where "$3+$" means that 3 is to be added to every element of the list. From this data we conjecture that

$$g_4(n) = 3 + \nu_2(n), \tag{7.69}$$

so that the (conjectured) integer

$$g_5(n) := \frac{g_4(n)}{2^{3+\nu_2(n)}} \tag{7.70}$$

is odd.

We now continue this process and examine the number $\nu_3(g_5(n))$. It seems that $g_5(n)$ is divisible by 3 for $n \geq 5$, so we consider

$$g_6(n) = \nu_3(g_5(n)). \tag{7.71}$$

Extensive symbolic calculations show that, for $i \geq 2$, we have

$$g_6(3i-1) = g_6(3i) = g_6(3i+1). \tag{7.72}$$

We pause our experiment here. The reader is invited to continue this exploration and begin proving some of these results.

The method outlined here is referred to by us as the *peeling strategy*: Given an expression for which we desire a closed-form, we use a symbolic language to peel away recognizable parts. The process ends successfully if one is able to reduce the original expression to a known one.

7.6 A Formula Hidden in the List

It is impossible for a table of integrals to be complete. In the process of studying integrals of rational functions, and after completing our study of Wallis' formula, we consider the integral

$$N_{0,4}(a;m) := \int_0^\infty \frac{dx}{(x^4+2ax^2+1)^{m+1}}. \tag{7.73}$$

We were surprised not to find it in [149]. The table does contain formula 3.252.11,

$$\begin{aligned}&\int_0^\infty (1+2\beta x+x^2)^{\mu-\frac{1}{2}} x^{-\nu-1}\,dx \\ &\quad = 2^{-\mu}(\beta^2-1)^{\mu/2}\Gamma(1-\mu)B(\nu-2\mu+1,-\nu)P^{\mu}_{\nu-\mu}(\beta),\end{aligned} \tag{7.74}$$

where B is the *Beta function*

$$B(x,y) := \int_0^1 t^{x-1}(1-t)^{y-1}\,dt = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} \tag{7.75}$$

and P_ν^μ is the *associated Legendre function*. We will not discuss here the technical details required to prove this. Using an appropriate representation of these functions, we showed that

$$P_m(a) := \frac{1}{\pi} 2^{m+3/2} (a+1)^{m+1/2} N_{0,4}(a;m) \tag{7.76}$$

is a polynomial in a, given by

$$P_m(a) = 2^{-2m} \sum_{k=0}^{m} 2^k \binom{2m-2k}{m-k} \binom{m+k}{m} (a+1)^k. \tag{7.77}$$

The reader will find the details in [41]. It turns out that this was not the original approach we followed to establish (7.76). At the time, we were completely unaware of the *hypergeometric world* involved in (7.74). Instead we used

$$\int_0^\infty \frac{dx}{bx^4 + 2ax^2 + 1} = \frac{\pi}{2\sqrt{2}} \frac{1}{\sqrt{a+\sqrt{b}}} \tag{7.78}$$

to produce in [42] the expansion

$$\sqrt{a+\sqrt{1+c}} = \sqrt{a+1} + \frac{1}{\pi\sqrt{2}} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} N_{0,4}(a;k-1) c^k. \tag{7.79}$$

The expression for $P_m(a)$ was a corollary of the Ramanujan Master Theorem; see [33] for details on this and many other results of Ramanujan. It was a long detour, forced by ignorance of a subject. It was full of surprises.

The coefficients of the polynomial $P_m(a)$ are given by

$$d_l(m) = 2^{-2m} \sum_{k=l}^{m} 2^k \binom{2m-2k}{m-k} \binom{m+k}{m} \binom{k}{l} \tag{7.80}$$

and have many interesting properties. Many of these we discovered by "playing around" with them on a computer.

For example, the sequence $\{d_l(m) : 0 \le l \le m\}$ is *unimodal*. That is, there is an index l^* such that $d_i(m) \le d_{i+1}(m)$ if $0 \le i \le l^* - 1$, and the inequality is reversed if $l^* \le i \le m$. In our study of $d_l(m)$, we discovered a general unimodality criteria. The details are presented in [5] and [40]. A property stronger than unimodality is that of *log-concavity*: a sequence of numbers $\{a_l\}$ is called log-concave if it satisfies $a_l^2 \ge a_{l-1}a_{l+1}$; see also Example 1.8. We have conjectured that the coefficients $d_l(m)$ are log-concave, but so far we have not been able to prove this.

As another example, the representation (7.80) provides an efficient way to compute $d_l(m)$ for m fixed if l is large relative to m. Trying to produce an alternative form that would give an efficient way to compute them when l is small, we established in [45] the existence of two families of polynomials $\alpha_l(m)$ and $\beta_l(m)$ such that

$$d_l(m) = \frac{1}{l!\,m!\,2^{m+l}}\left(\alpha_l(m)\prod_{k=1}^{m}(4k-1) - \beta_l(m)\prod_{k=1}^{m}(4k+1)\right). \tag{7.81}$$

The degrees of α_l and β_l are l and $l-1$, respectively. For instance, the linear coefficient of $P_m(a)$ is given by

$$d_1(m) = \frac{1}{m!\,2^{m+1}}\left((2m+1)\prod_{k=1}^{m}(4k-1) - \prod_{k=1}^{m}(4k+1)\right), \tag{7.82}$$

and the quadratic one is

$$d_2(m) = \frac{1}{m!\,2^{m+2}}\left((2m^2+2m+1)\prod_{k=1}^{m}(4k-1) - (2m+1)\prod_{k=1}^{m}(4k+1)\right).$$

On a day without new ideas,[4] we started computing zeroes of the polynomials α_l and β_l. We were very surprised to see that *all of them* were on the vertical line $\text{Re}\, m = -\frac{1}{2}$. In the summer of 2002, while working at SIMU (Summer Institute in Mathematics for Undergraduates), we had a good idea about how to solve this problem: Ask John Little. The result is true. The polynomial $A_l(s) := \alpha_l(\frac{s-1}{2})$ satisfies the recurrence

$$A_{l+1}(s) = 2sA_l(s) - (s^2 - (2l-1)^2)A_{l-1}(s), \tag{7.83}$$

and the location of the zeroes can be deduced from here. The details appear in [201].

This example illustrates our working philosophy: There are many classes of definite integrals that have very interesting mathematics hidden in them. The use of a symbolic language often helps you find the correct questions.

The logconcavity of the coefficients $d_l(m)$ has been recently established by M. Kauers and P. Paule [177]. Using the RISC package MultiSum [276], they show that the triple sum

$$d_l(m) = \sum_{j,s,k} \frac{(-1)^{k+j-l}}{2^{3(k+3)}}\binom{2m+1}{2s}\binom{m-s}{k}\binom{2(k+s)}{k+s}\binom{s}{j}\binom{k}{l-j}$$

satisfies the recurrence

[4] Like most of them.

$$-2(l+m)d_{l-1}(m)-(2l+4m+3)d_l(m)+2(m+1)d_l(m+1)=0.$$

This provides a computer-generated proof of the positivity of $d_l(m)$.

Christian Mallinger's package `GeneratingFunctions.m` is used to prove that the polynomials $P_m(a)$ are nothing but special instances of Jacobi polynomials. A classical proof of this result appears in [41].

The authors then employ methods of cylindrical algebra decomposition [82, 94] to show that the logconcavity of $d_l(m)$ follows from the inequality

$$d_l(m+1) \geq \frac{p_1(l,m)+\sqrt{p_2(l,m)}}{p_3(l,m)} d_l(m), \tag{7.84}$$

for (l,m) in a certain region of $\mathbb{Z}^2$ and

$$\begin{aligned} p_1(l,m) &= -2l^2+(m+1)(4m+3), \\ p_2(l,m) &= l(4l^3-3l-4m(m+1)), \\ p_3(l,m) &= 2(m+1)(m-l+1). \end{aligned}$$

The inequality (7.84) is replaced by the stronger condition

$$d_l(m+1) \geq \frac{4m^2+7m+l+1}{2(m+1-l)(m+1)} d_l(m). \tag{7.85}$$

This is established using the RISC package SumCracker developed by M. Kauers [176].

7.7 Some Experiments on Valuations

We now report on some experiments concerning the p-adic valuation of the coefficients $d_l(m)$ defined in the previous section. The expression

$$d_l(m) = 2^{-2m} \sum_{k=l}^{m} 2^k \binom{2m-2k}{m-k} \binom{m+k}{m} \binom{k}{l} \tag{7.86}$$

shows that $\nu_p(d_l(m)) \geq 0$ for $p \neq 2$.

We now describe results of symbolic calculations of the p-adic valuation of

$$f(m,l) = \alpha_l(m) \prod_{k=1}^{m}(4k-1) - \beta_l(m) \prod_{k=1}^{m}(4k+1). \tag{7.87}$$

The coefficients $d_l(m)$ and $f(m,l)$ are related via $f(m,l) = l!m!2^{m+l}d_l(m)$. These two functions are computationally equivalent because the p-adic valuations of factorials are easily computed via

$$\nu_p(m!) = \sum_{k=1}^{\infty} \left\lfloor \frac{m}{p^k} \right\rfloor. \tag{7.88}$$

Naturally, the sum is finite and we can end it at $k = \lfloor \log_p m \rfloor$. An alternative is to use a famous result of Legendre [194, 150],

$$\nu_p(m!) = \frac{m - s_p(m)}{p-1}, \tag{7.89}$$

where $s_p(m)$ is the sum of the base-p digits of m.

The command

```
g[m_,l_,p_]:= IntegerExponent[ f[m,l],p ]
```

gives directly the p-adic valuation of the coefficient $f(m,l)$. For example, for $m = 30, l = 10$, and $p = 3$, we have $g(30,10,3) = 18$. Indeed,

$$f(30,10) = 2^{30} \cdot 3^{18} \cdot 5^{10} \cdot 7^6 \cdot 11^4 \cdot 13^3 \cdot 17^2 \cdot 19^2 \cdot 23^2 \cdot N, \tag{7.90}$$

where N is the product of five primes.

We have evaluated the function $g(m,l,p)$ for large classes of integers m, l and primes p.

The remainder of this section describes our findings. The situation is quite different according to whether $p = 2$ or p is odd. In the first case, $g(m,l,2)$ has a well-defined structure. In the latter, $g(m,l,p)$ has a random flavor. In this case we have only been able to predict its asymptotic behavior.

7.7.1 The Case $p = 2$

The experiments show that, for fixed l, the function $g(m,l,2)$ has blocks of length $2^{\nu_2(l)+1}$. For example, the values of $g(m,1,2)$ for $1 \leq m \leq 20$ are

$$\{2,2,3,3,2,2,4,4,2,2,3,3,2,2,5,5,2,2,3,3\}.$$

Similarly, $g(m,4,2)$ has blocks of length 8: It begins with eight 11's, followed by eight 12's, continued by eight 11's, and so on. The graphs of some functions $g(m,l,2)$, where we reduced the repeating blocks to a single value, are shown in Figures 7.2–7.5.

The main experimental result is that the graph of $g(m,l,p)$ has an *initial segment* from which the rest is determined by adding a *central piece* followed by a

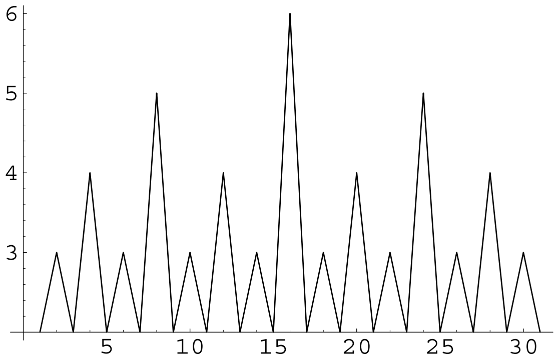


Figure 7.1. The 2-adic valuation of $d_1(m)$.

folding rule. For example, in the case $l = 1$, the first few values of the reduced table for $g(m,1,2)$ are

$$\{2, 3, 2, 4, 2, 4, 2, 3, 2, 5, \ldots\}.$$

The ingredients are

- **Initial segment.** $\{2, 3, 2\}$.
- **Central piece.** The value at the center of the initial segment, namely 3.
- **Rules of formation.** Start with the initial segment, and add 1 to the central piece and reflect.

This produces the sequence

$$\{2,3,2\} \to \{2,3,2,4\} \to \{2,3,2,4,2,3,2\} \to \{2,3,2,4,2,3,2,5\}$$

$$\to \{2,3,2,4,2,3,2,5,2,3,2,4,2,3,2\}.$$

The details are shown in Figure 7.1.

The difficulty with this procedure is that, at the moment, we have no form of determining the initial segment nor the central piece. Figure 7.2 shows the beginning of the function $g(m,9,2)$. From here one could be tempted to predict that this graph extends as in the case $l = 1$. This is not correct, as can be seen in Figure 7.3. The new pattern shown in Figure 7.4 seems to be the correct one.

The initial pattern could be quite elaborate. Figure 7.5 illustrates the case $l = 53$.

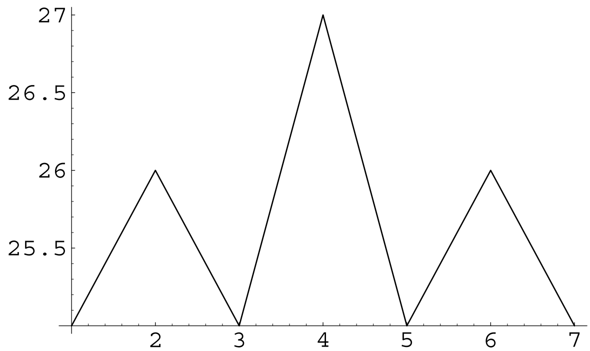


Figure 7.2. The beginning of $g(m, 9, 2)$.

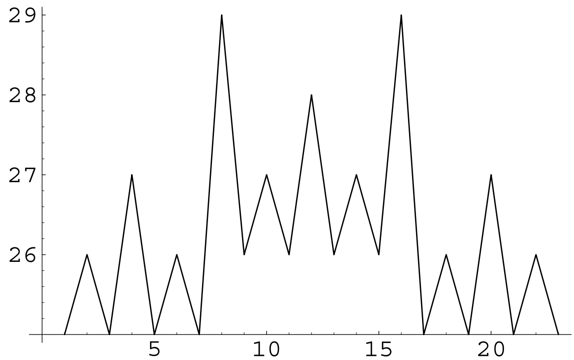


Figure 7.3. The continuation of $g(m, 9, 2)$.

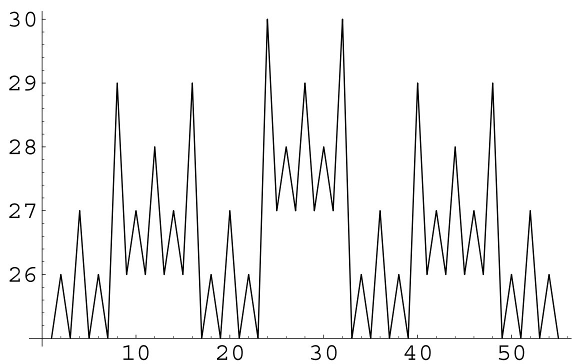


Figure 7.4. The pattern of $g(m, 9, 2)$ persists.

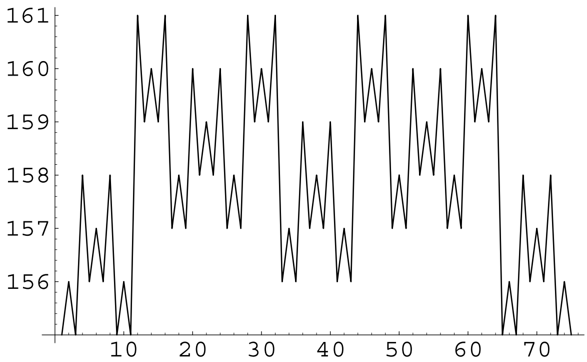


Figure 7.5. The initial pattern for $l = 53$.

In [45] we have given details of the following result: The 2-adic valuation of $d_1(m)$ is given by

$$\nu_2(d_1(m)) = 1 - m + \nu_2\left(\binom{m+1}{2}\right) - \nu_2(m!). \tag{7.91}$$

This has been extended in [208] where we have established

$$\nu_2(A_{l,m}) = \nu_2((m+1-l)_{2l}) + l, \tag{7.92}$$

where $(m)_k$ is the Pochhammer symbol and $A_{l,m} = l!m!2^{m+l}d_l(m)$.

7.7.2 The Case of Odd Primes

The p-adic valuation of $d_l(m)$ behaves quite differently for p an odd prime. Figure 7.6 shows the values for $l = 1$ and $p = 3$. There is a clear linear growth, of slope $\frac{1}{2}$, and Figure 7.7 shows the deviation from this linear function. We suspect that the error is bounded.

This behavior persists for other values of l and primes p. The p-adic valuation of $d_l(m)$ has linear growth with slope $1/(p-1)$. Figures 7.8–7.11 show four representative cases.

Conjecture 7.1. *Let p be an odd prime. Then*

$$\nu_p(d_l(m)) \sim \frac{m}{p-1}. \tag{7.93}$$

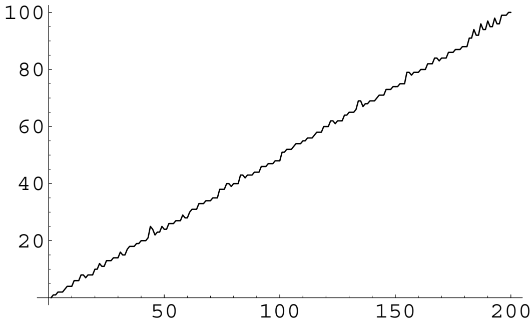


Figure 7.6. The 3-adic valuation of $d_1(m)$.

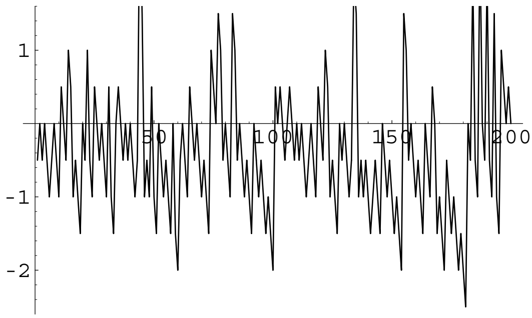


Figure 7.7. The deviation from linear growth.

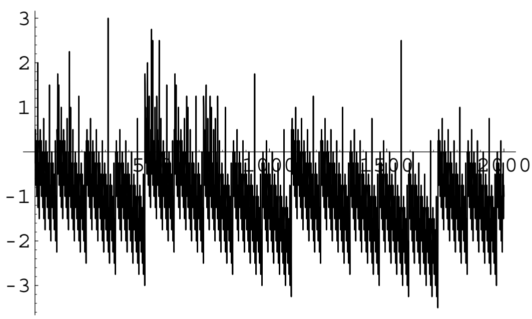


Figure 7.8. The error for $l = 1$ and $p = 5$.

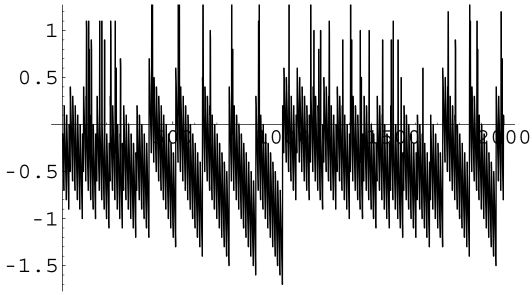


Figure 7.9. The error for $l = 1$ and $p = 11$.

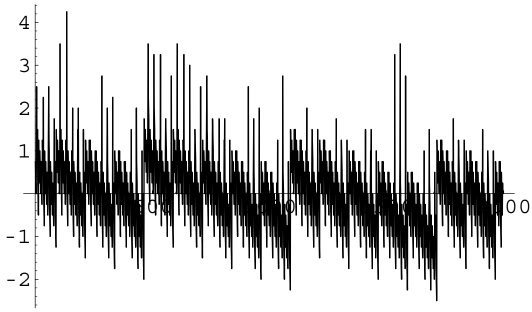


Figure 7.10. The error for $l = 5$ and $p = 5$.

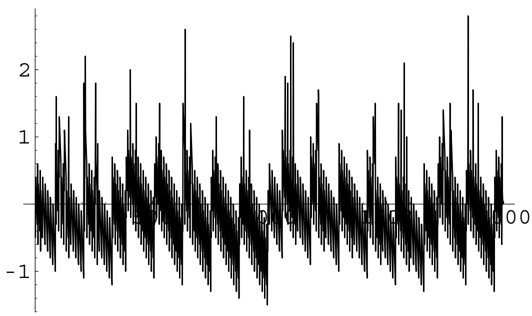


Figure 7.11. The error for $l = 5$ and $p = 11$.

7.8 An Error in the Latest Edition

A project of the size of [149] is bound to have some errors. In the last edition of the table, we found formula 3.248.5 as a new addition to this great collection. It has a beautiful structure given by nested radicals. Let

$$\varphi(x) = 1 + \frac{4x^2}{3(1+x^2)^2}; \tag{7.94}$$

then, the evaluation states that

$$\int_0^\infty \frac{dx}{(1+x^2)^{3/2}\left[\varphi(x)+\varphi(x)^{1/2}\right]^{1/2}} = \frac{\pi}{2\sqrt{6}}. \tag{7.95}$$

After several failed attemps at proving it, we decided to check it numerically. *It is incorrect.*[5] Normally this is disappointing, but in this case the structure of the evaluation leads to two interesting problems:

- **The direct problem.** Find the correct value of the integral. As usual there is no method that is guaranteed to succeed, and a good idea is required.
- **The inverse problem.** Given that $\pi/2\sqrt{6}$ is the correct answer, find a modification of the integrand that produces that answer. This modification is expected to be close to the integrand given in the table, perhaps a typo: The exponent $\frac{3}{2}$ in the term $1+x^2$ perhaps is $\frac{2}{3}$; or the 4 in the expression for $\varphi(x)$ is a 14. There is no systematic approach to solving this problem, but it is a lot of fun to experiment with it.

We have not explored this example in detail, but it seems to have many beautiful alternative representations. For instance, let

$$a[x,p] := \sqrt{x^4+2px^2+1}. \tag{7.96}$$

Then, the integral is $I(\frac{5}{3},1)$, where

$$I(p,q) = \int_0^\infty \frac{dx}{a[x,p]^{1/2}a[x,q]^{1/2}(a[x,p]+a[x,q])^{1/2}}. \tag{7.97}$$

It is interesting to observe that if

$$b[x,p] := \sqrt{x^2+2px+1}, \tag{7.98}$$

then the integral is $J(\frac{5}{3},1)$, where

$$J(p,q) = \frac{1}{2}\int_0^\infty \frac{dx}{b[x,p]^{1/2}b[x,q]^{1/2}(b[x,p]+b[x,q])^{1/2}}. \tag{7.99}$$

[5] We should have checked earlier.

7.9 Some Examples Involving the Hurwitz Zeta Function

There are many evaluations in [149] where the Hurwitz zeta function

$$\zeta(z,q) = \sum_{k=0}^{\infty} \frac{1}{(k+q)^z} \tag{7.100}$$

appears as part of the value of the integral. For example, entry 3.524.1 states that

$$\int_0^\infty x^{\mu-1} \frac{\sinh \beta x}{\sinh \gamma x}\, dx = \frac{\Gamma(\mu)}{(2\gamma)^\mu} \left\{ \zeta \left[\mu, \frac{1}{2}\left(1 - \frac{\beta}{\gamma}\right)\right] - \zeta \left[\mu, \frac{1}{2}\left(1 + \frac{\beta}{\gamma}\right)\right] \right\}$$

is valid for $\operatorname{Re}\gamma > |\operatorname{Re}\beta|$ and $\operatorname{Re}\mu > -1$. The identity (7.101) can be written in the *typographically* simpler form

$$\int_0^\infty x^{\mu-1} \frac{\sinh bx}{\sinh x}\, dx = \frac{\Gamma(\mu)}{2^\mu} \left\{ \zeta \left[\mu, \frac{1}{2}(1-b)\right] - \zeta \left[\mu, \frac{1}{2}(1+b)\right] \right\},$$

which illustrates the fact that entry 3.524.1 has only two independent parameters.

The table [149] contains no examples in which $\zeta(z,q)$ appears in the integrand. A search of the three-volume compendium [242] produces

$$\int \zeta(z,q)dq = \frac{1}{1-z}\zeta(z-1,q), \tag{7.101}$$

which is an elementary consequence of

$$\frac{\partial}{\partial q}\zeta(z-1,q) = (1-z)\zeta(z,q), \tag{7.102}$$

and in [242, Section 2.3.1], we find the moment

$$\int_0^\infty q^{\alpha-1}\zeta(z,a+bq)dq = b^{-\alpha}B(\alpha,z-\alpha)\zeta(z-\alpha,a). \tag{7.103}$$

Motivated mostly by the lack of explicit evaluations, we initiated in [129, 130] a systematic study of these type of integrals. Our results are based mostly on the expressions for the Fourier coefficients of $\zeta(z,q)$ given in [242, Section 2.3.1] as

$$\int_0^1 \sin(2\pi q)\zeta(z,q)dq = \frac{(2\pi)^z}{4\Gamma(z)} \csc\left(\frac{z\pi}{2}\right). \tag{7.104}$$

Some interesting evaluations are obtained from Lerch's identity,

$$\frac{d}{dz}\zeta(z,q)|_{z=0} = \log\Gamma(q) - \log\sqrt{2\pi}. \tag{7.105}$$

For instance, the reader will find in [129] the elementary value

$$\int_0^1 \log\Gamma(q)dq = \log\sqrt{2\pi} \tag{7.106}$$

and the surprising value

$$\int_0^1 (\log\Gamma(q))^2\,dq = \frac{\gamma^2}{12} + \frac{\pi^2}{48} + \frac{1}{3}\gamma\log\sqrt{2\pi} + \frac{4}{3}\left(\log\sqrt{2\pi}\right)^2 - (\gamma + 2\log\sqrt{2\pi})\frac{\zeta'(2)}{\pi^2} + \frac{\zeta''(2)}{2\pi^2}. \tag{7.107}$$

An elementary proof of (7.106), due to T. Amdeberhan, uses only the elementary properties of the Gamma function. The first step is to partition the interval $[0,1]$ to obtain

$$\int_0^1 \log\Gamma(x)\,dx = \lim_{n\to\infty} \frac{1}{n}\sum_{k=1}^{n} \log\Gamma(k/n). \tag{7.108}$$

The Riemann sum can be written as

$$\begin{aligned} \frac{1}{n}\sum_{k=1}^{n}\log\Gamma(k/n) &= \frac{1}{n}\log\left(\prod_{k=1}^{n}\Gamma\left(\tfrac{k}{n}\right)\right) \\ &= \frac{1}{n}\log\left(\prod_{k=1}^{n/2}\Gamma\left(\tfrac{k}{n}\right)\Gamma\left(1-\tfrac{k}{n}\right)\right), \end{aligned}$$

and using the reflection formula (7.7) we obtain

$$\frac{1}{n}\sum_{k=1}^{n}\log\Gamma(k/n) = \log\sqrt{\pi} - \log\left(\prod_{k=1}^{n/2}\sin(\pi k/n)\right)^{1/n}. \tag{7.109}$$

The identity

$$\prod_{k=1}^{n-1}\sin\left(\frac{\pi k}{n}\right) = \frac{n}{2^{n-1}} \tag{7.110}$$

written as

$$\left(\prod_{k=1}^{n/2}\sin\left(\frac{\pi k}{n}\right)\right)^{1/n} = \frac{(2n)^{1/2n}}{\sqrt{2}} \tag{7.111}$$

yields the evaluation.

We now observe that, for $n=1$ and $n=2$, the integral

$$LG_n := \int_0^1 (\log\Gamma(q))^n\,dq \tag{7.112}$$

is a homogeneous polynomial of degree n in the variables γ, π, $\log\sqrt{2\pi}$, $\zeta(2)$, $\zeta'(2)$, and $\zeta''(2)$. This is similar to (7.21). In this problem the weights are assigned experimentally as follows:

- The weight of a rational number is 0.
- The constants π, γ have weight 1 and so does $\log\sqrt{2\pi}$, that is,

$$w(\pi) = w(\gamma) = w(\log\sqrt{2\pi}) = 1. \tag{7.113}$$

- The weight is extended as $w(ab) = w(a) + w(b)$.
- The value $\zeta(j)$ has weight j, so that $w(\zeta(2)) = 2$ is consistent with $\zeta(2) = \pi^2/6$.
- Differentiation increases the weight by 1, so that $\zeta''(2)$ has weight 4.

We have been unable to evaluate the next example,

$$LG_3 := \int_0^1 (\log\Gamma(q))^3 \, dq, \tag{7.114}$$

but in our (failed) attempts we have established [131] a connection between LG_n and the *Tornheim-Zagier sums* (or *Witten ζ-functions*)

$$T(a,b;c) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{1}{n^a m^b (n+m)^c}. \tag{7.115}$$

These sums will reappear in Chapter 8. An extensive bibliography on these *multiple zeta series* has been compiled by M. Hoffman [169].

In our current work, we have been able to express the sums $T(a,b;c)$ in terms of integrals of triple products of the Bernoulli polynomials and the function

$$A_k(q) = k\zeta'(1-k,q). \tag{7.116}$$

The classical identity

$$B_k(q) = -k\zeta(1-k,q) \tag{7.117}$$

shows the similarity between A_k and B_k.

This is just one more example of the beautiful mathematics that one is able to find by experimenting with integrals.

8 Experimental Mathematics: A Computational Conclusion

Mathematicians are like a certain type of Frenchman: when you talk to them they translate it into their own language and then it soon turns into something entirely different.[1]

—Johann Wolfgang von Goethe [147, Maxim 1279]

8.1 Mathematicians Are a Kind of Frenchmen

We have now seen experimental, computationally assisted mathematics in action in areas pure and applied, discrete and continuous. In each case perhaps Goethe said it best in the above quote. Goethe was right, and we do it to wonderful effect. Returning however to views about the nature of mathematics, Greg Chaitin takes things much further than Gödel did.

> Over the past few decades, Gregory Chaitin, a mathematician at IBM's T. J. Watson Research Center in Yorktown Heights, N.Y., has been uncovering the distressing reality that much of higher math may be riddled with unprovable truths—that it's really a collection of random facts that are true for no particular reason. And rather than deducing those facts from simple principles, "I'm making the suggestion that mathematics is done more like physics in that you come about things experimentally," he says. "This will still be controversial when I'm dead. It's a major change in how you do mathematics." (*Time Magazine*, Sept 4, 2005)

Chaitin was featured in a brief article, "The Omega Man," which is also the name of his new book on computational complexity.

This "Ω" refers to Chaitin's seminal halting probability constant [85]

$$\Omega := \sum_{\pi} 2^{-\#(\pi)},$$

where π ranges over halting Turing machines and $\#(\pi)$ is its length. While intrinsically noncomputable and *algorithmically irreducible*, the first 64 bits are

[1] *"Die Mathematiker sind eine Art Franzosen: Redet man zu ihnen, so übersetzen sie es in ihre Sprache, und dann ist es alsobald ganz etwas anders."*

provably known:

$$\Omega := 0.000000100000010000100000100001110111001100100111100010010011100\ldots$$

"Most of mathematics is true for no particular reason," Chaitin says. "Maths is true by accident."

8.1.1 History of Computer Experiments

A reviewer of [50] and [51] made the observation that there were a significant number of early discussions of computer-assisted mathematics not referenced in those books. While we were aware of many of them such as [195] and Tymoczko's well-known writings on the four color theorem [269, 270], others were not familiar to us but certainly deserve recording, such as [34, 138, 290].

More broadly in the context of scientific discovery, the Nobel economist Herbert Simon reflects generally on the current and future power of computer-generated scientific discovery. When asked "Do you have a guess when a computer will make a Nobel-worthy discovery?" he replies, "I'm pausing to think if that's already happened." [259] He then goes on to describe how his program *BACON* rediscovered Kepler's third law and the power of programs such as *MECHCHEM* to study chemical reactions.

With or without computers, it is difficult to capture what is involved in research. Consider the response of Dr. Edward Witten of the Institute for Advanced Study in Princeton, New Jersey when asked by CNN what he does all day:

> There isn't a clear task. If you are a researcher you are trying to figure out what the question is as well as what the answer is.
>
> You want to find the question that is sufficiently easy that you might be able to answer it, and sufficiently hard that the answer is interesting. You spend a lot of time thinking and you spend a lot of time floundering around.[2]

8.2 Putting Lessons in Action

In "Proof and Beauty," the *Economist* of March 31, 2005 wrote,

> Just what does it mean to prove something? Although the *Annals* will publish Dr Hales's paper, Peter Sarnak, an editor of the *Annals*,

[2] Witten was interviewed on CNN June 27, 2005.

whose own work does not involve the use of computers, says that the paper will be accompanied by an unusual disclaimer, stating that the computer programs accompanying the paper have not undergone peer review. There is a simple reason for that, Dr Sarnak says—it is impossible to find peers who are willing to review the computer code. However, there is a flip-side to the disclaimer as well—Dr Sarnak says that the editors of the *Annals* expect to receive, and publish, more papers of this type—for things, he believes, will change over the next 20–50 years. Dr Sarnak points out that maths may become "a bit like experimental physics" where certain results are taken on trust, and independent duplication of experiments replaces examination of a colleague's paper.

Why should the non-mathematician care about things of this nature? The foremost reason is that mathematics is beautiful, even if it is, sadly, more inaccessible than other forms of art. The second is that it is useful, and that its utility depends in part on its certainty, and that that certainty cannot come without a notion of proof. Dr Gonthier, for instance, and his sponsors at Microsoft, hope that the techniques he and his colleagues have developed to formally prove mathematical theorems can be used to "prove" that a computer program is free of bugs—and that would certainly be a useful proposition in today's software society if it does, indeed, turn out to be true.

8.3 Visual Computing

In a similar light *visual computing* is in its infancy, and we can only imagine its future, but already there are many interesting harbingers both theoretical and applied.

8.3.1 The Perko Pair

In many knot compendia produced since the nineteenth century, the first two knots in Figure 8.1 below have been listed as distinct ten crossing knots. They were however shown to be the same by Ken Perko in 1974. This is best illustrated dynamically in a program like *Knotplot* which will diffeomorphically adjust both into the third knot.

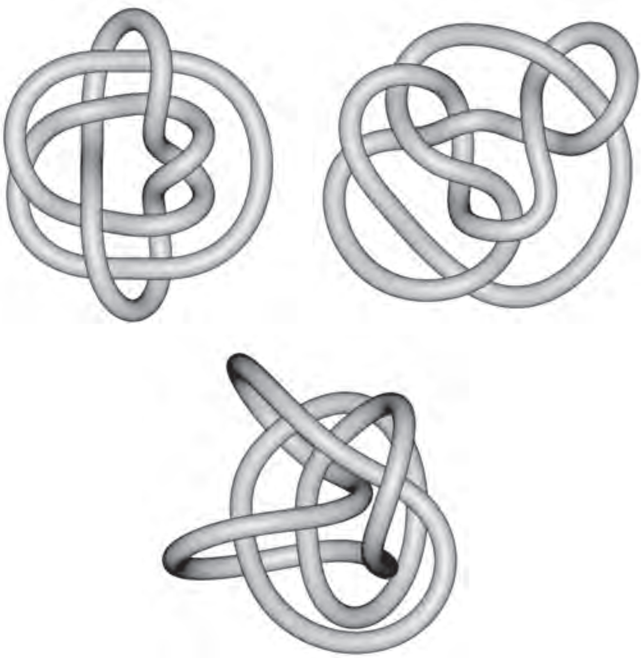


Figure 8.1. The Perko Pair of Knots.

8.3.2 Fractal Cards and Chaos Games

Deterministic Constructions. Not all impressive discoveries require a computer. Elaine Simmt and Brent Davis [254] describe lovely constructions made by repeated regular paper folding and cutting—but no removal of paper—that result in beautiful fractal, self-similar, "pop-up" cards.

Nonetheless, in Figures 8.2 and 8.3 we choose to show various iterates of a pop-up Sierpiński triangle built in software, on turning those paper cutting and folding rules into an algorithm given in [50, pp. 94–95]. This should be enough to let one start folding.

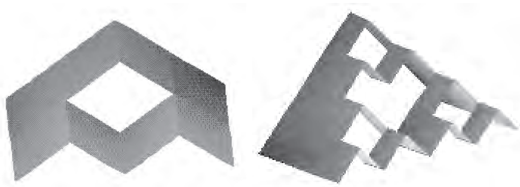


Figure 8.2. The first and second iterates of a Sierpiński card.

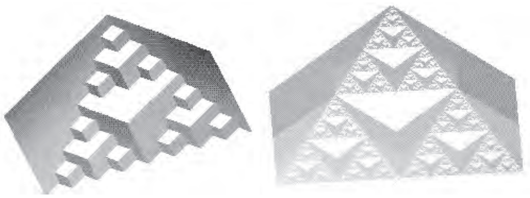


Figure 8.3. The third and seventh iterates of a Sierpiński card.

Note the similarity to the Pascal triangles given in Figure 8.4. This is clarified when we note the pattern modulo two with the even numbers in boldface:

1
1 1
1 **2** 1
1 3 3 1
1 **4** **6** **4** 1
1 5 **10** **10** 5 1
1 **6** 15 **20** 15 **6** 1
1 7 21 35 35 21 7 1
⋮

One may consider more complex modular patterns as discussed in Andrew Granville's online paper on binomial coefficients [151]. Likewise, we draw the reader's attention to the recursive structures elucidated in the chapter on strange

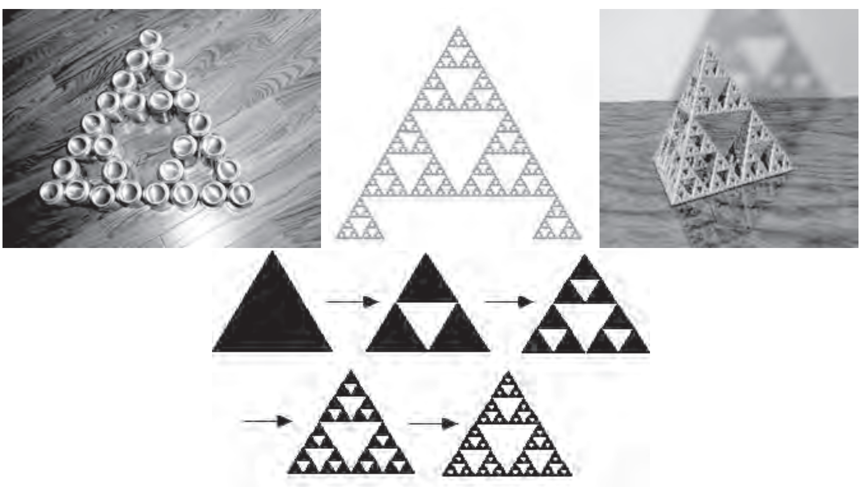


Figure 8.4. Pascal's Triangle modulo two above a Sierpiński construction.

Figure 8.5. Self-similarity in Chartres and Granada.

functions. And always, art can be an additional source of mathematical inspiration and stimulation, as in the rose window from Chartres and the view of the Alhambra in Granada shown in Figure 8.5.

Random Constructions. These prior constructions are all deterministic and so relate closely to the ideas about cellular automata discussed at length in Stephen Wolfram's *A New Kind of Science*. But, as we shall see, random constructions lead naturally to similar self-replicative structures.

In [50, §2.4] we described how to experimentally establish that we do indeed obtain a Sierpiński triangle from Pascal's triangle and noted also that simple random constructions led to the Sierpiński triangle or *gasket*: Construct an arbitrary triangle, with vertices $(x_1,y_1),(x_2,y_2)$, and (x_3,y_3). Specify a point (x,y) within the triangle. Then, iterate indefinitely the following construction: First select a random integer r in the set $(1,2,3)$, and then construct a new point (x',y') as follows:

$$(x',y') \quad = \quad \left(\frac{1}{2}(x+x_r),\frac{1}{2}(y+y_r)\right). \tag{8.1}$$

The corresponding graph will yield a Sierpiński gasket asymptotically, as we see below. Even more intriguing is the following link with genetic processes.

8.4 A Preliminary Example: Visualizing DNA Strands

Suppose that we have a strand of DNA, that is, a string whose elements may be any of four symbols (bases): A (adenosine), C (cytosine), G (guanine), or T (thymine).

ATGGACTTCCAG (8.2)

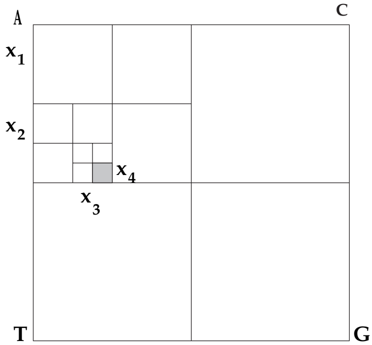


Figure 8.6. Visualizing DNA sequences of length n.

Each DNA sequence can be identified with a unique sub-square in the unit square $[0,1] \times [0,1]$ as follows: Identify each base, A, C, G, and T, with a vertex of the square (see Figure 8.6). Let x_n denote the sub-square corresponding to the subsequence of length n, and let ω_n be the nth base. With each iteration, we will subdivide the square into four smaller squares. The initial region x_0 is the entire unit square. Given x_{n-1}, calculate the next region x_n as follows.

1. Find the nth base ω_n in the sequence.

2. Subdivide the square x_{n-1} into four smaller squares. Set x_n to be the sub-square of x_{n-1} closest to the vertex ω_n. That is, if $\omega_n = \text{A}$, then x_n is the upper left sub-square of x_{n-1}; if $\omega_n = \text{G}$, then x_n is the lower right sub-square of x_{n-1}.

3. Plot x_n as follows. Replace x_{n-1} with the square x_{n-1} subdivided into four smaller squares, and shade in the sub-square x_n.

The first few sub-squares x_n, corresponding to the subsequences of length n of the sequence in (8.2), are shown in Figure 8.6. Note that different sequences yield distinct sub-squares in $[0,1] \times [0,1]$, with a one-to-one correspondence between dyadic sub-squares of the unit square and finite sequences of DNA.

Here we iterate a simple algorithm that calculates a new x_n from the previous x_{n-1}, plus an additional piece of information (ω_n), and displays the x_n graphically. As we describe below, this is the main idea behind the *chaos game*.

8.5 What Is a Chaos Game?

A *chaos game* is a probabilistic algorithm for visualizing the *attractor* of an *iterated function system*. Chaos games can be used to generate fractals, since in many cases the attractor of an iterated function system is a fractal.

What does this mean? Suppose that we are working in a metric space X, say $X = \mathbb{R}^2$, and we have a finite collection $\{w_i\}_{i=1}^N$ of contractive maps $w_i : X \to X$. The pair $(X, \{w_i\}_{i=1}^N)$ is called an *iterated function system* (IFS). A basic proposition in the study of dynamical systems states that there exists a unique nonempty compact set $A \subset X$ such that

$$A = \bigcup_{i=1}^{N} w_i(A),$$

and if we define $S_n := \bigcup_{i=1}^N w_i(S_{n-1})$ for an arbitrary nonempty compact set $S_0 \subset X$, the Hausdorff distance

$$h(S_n, A) \to 0$$

as $n \to \infty$ (that is, S_n converges to A in the Hausdorff metric[3]). The set A is called the *attractor* of the iterated function system $(X, \{w_i\}_{i=1}^N)$. If $X = \mathbb{R}$ or $X = \mathbb{R}^2$, we can choose some compact set S_0 and graph the sets S_n for successively larger and larger n to visualize successively better approximations to the attractor A. The chaos game algorithm gives a different method for visualizing the attractor.

To set up a chaos game, we first must associate a probability p_i with each of the contractive mappings w_i in our iterated function system. That is, $0 \leq p_i \leq 1$ for each i and $\sum_{i=1}^N p_i = 1$. In each iteration of the chaos game algorithm, we will select one of the maps w_i randomly, with p_i being the probability of selecting map w_i. The triple $(X, \{w_i\}_{i=1}^N, \{p_i\}_{i=1}^N)$ is called an *iterated function system with probabilities* (IFSP).

Algorithm 8.1 (Chaos Game Algorithm). Initialize by selecting a fixed point $x_0 \in X$ of one of the maps, say w_1.
Plot x_0.
Iterate until a preassigned number of steps is reached:

1. Select a map w_{i_n} at random according to the probabilities p_i.
2. Set $x_n = w_{i_n}(x_{n-1})$.
3. Plot x_n.

When using this algorithm to visualize an attractor of an IFSP, we will stop after a preset maximum number of iterations or when nothing new is added on our computer screen anymore (because the attractor has already filled out).

[3] Remember that $h(A,B) := \inf\{r : A \subseteq N_r(B) \text{ and } B \subseteq N_r(A)\}$ is a metric on the set of nonempty compact subsets of X, the *Hausdorff metric*. Here $N_r(A) := \{y : d(x,y) < r \text{ for some } x \in A\}$ is the open r-neighborhood of A for $r > 0$.

Since the point x_0 is initialized to be in the attractor, all subsequent points x_n will also be in the attractor. Running the chaos game algorithm for a small number of iterations will give only the barest outline of the shape of the attractor. Eventually we fill in more detail, however. We can also start over after a finite number of iterations, reinitialize the chaos game, and plot additional points x'_n along a (probably) different trajectory, to add more detail to our plot of points in the attractor.

More information about chaos games and iterated function systems can be found in the papers by Mendivil and Silver [213] and by Ashlock and Golden [8], discussed further below.

8.5.1 Examples of Chaos Games

Example 8.2 (Sierpiński Triangle). The Sierpiński Triangle can be generated from an iterated function system with three maps:

$$\begin{aligned} w_1 &: x \mapsto \frac{x+v_1}{2}, \\ w_2 &: x \mapsto \frac{x+v_2}{2}, \\ w_3 &: x \mapsto \frac{x+v_3}{2}, \end{aligned}$$

where x is a point in $\mathbb{R}^2$, v_1 is the point $(0,1)$, v_2 is the point $(-1,0)$, and v_3 is the point $(0,\sqrt{3})$. (These are three vertices of an equilateral triangle in $\mathbb{R}^2$.) Each map w_i maps the current point x to a point halfway in between x and the vertex v_i. We will choose the maps w_i according to a uniform probability distribution, with $p_i = \frac{1}{3}$ for each i, to make an IFSP out of this iterated function system.

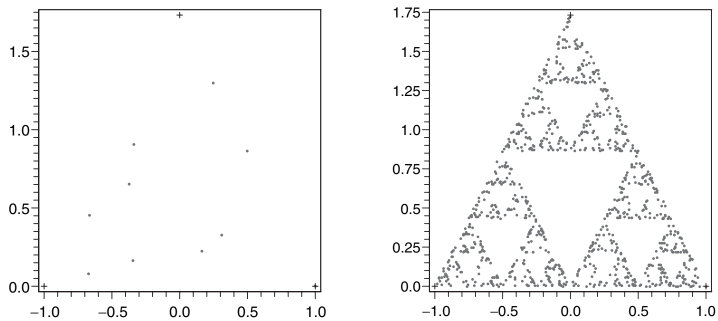


Figure 8.7. Chaos game for the Sierpiński Triangle after 10 and 1000 iterations.

For each i, the point v_i is a fixed point of the map w_i (e.g., $w_1(v_1) = \frac{v_1+v_1}{2} = v_1$), so we may initialize the chaos game by setting $x_0 := v_1$ and plotting x_0. Several iterations of the chaos game are shown in Figure 8.7. ◇

Example 8.3 (Twin Dragon). Let $d_0 = (0,0)$ and $d_1 = (1,0)$ be points in $\mathbb{R}^2$. Let M be the twin dragon matrix

$$M = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}.$$

Then the maps

$$w_1 : x \mapsto M^{-1}(x+d_0)$$
$$w_2 : x \mapsto M^{-1}(x+d_1)$$

form an iterated function system. We can assign the probabilities $p_1 = p_2 = \frac{1}{2}$ to the maps w_1 and w_2 to make an IFSP. Note that the origin $d_0 = (0,0)$ is a fixed point of the map w_1, thus we can initialize $x_0 := d_0 = (0,0)$ in the chaos game, and plot x_0. Several iterations are shown in Figure 8.8. ◇

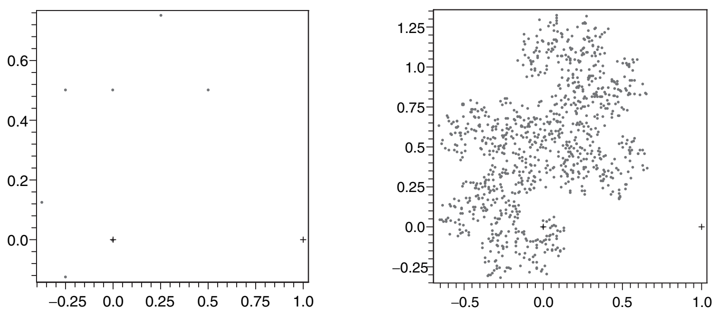


Figure 8.8. Chaos game for the Twin Dragon after 10 and 1000 iterations.

Example 8.4 (Strange Functions and Functional Equations). In Section 5.1 we described functional equations for nondifferentiable functions such as the Weierstrass functions. These functional equations can also be recast in terms of the chaos game. As in Section 5.1, assume $|a_0|, |a_1| < 1$ and $g_0, g_1 : [0,1] \to \mathbb{R}$. Define

$$w_1 : (x,y) \mapsto \left(\frac{x}{2}, a_0\, y + g_0(x)\right),$$
$$w_2 : (x,y) \mapsto \left(\frac{x+1}{2}, a_1\, y + g_1(x)\right).$$

Then, in the cases discussed in Section 5.1, where the system of functional equations (5.1)–(5.2) has a unique solution, the graph of this solution is precisely the attractor of the IFS $\left(\mathbb{R}^2, \{w_1, w_2\}\right)$. (See [32], where this correspondence is explored.)

In Section 5.1, we did not use a probabilistic algorithm (chaos game) to plot this graph but instead used a deterministic algorithm: The Banach iteration described there can be viewed as starting with the nonempty compact set

$$S_0 := \left\{ \left(0, \frac{g_0(0)}{1-a_0}\right), \left(1, \frac{g_1(1)}{1-a_1}\right) \right\}$$

(consisting of the fixed points of w_1, w_2) and computing the sets $S_n := w_1(S_{n-1}) \cup w_2(S_{n-1})$ successively. ◇

Example 8.5 (Scaling Functions and Wavelets). We follow the notation of Mendivil and Silver [213] in this section and present a simpler chaos-game algorithm here than is given in [213]. While Mendivil and Silver's algorithm can additionally be used in wavelet analysis and synthesis, our simplified algorithm suffices to visualize the scaling function and wavelet. A scaling function $\phi(x)$ for a *multiresolution analysis* satisfies a *scaling equation*

$$\phi(x) = \sum_{n\in\mathbb{Z}} h_n \phi(2x-n), \tag{8.3}$$

where the coefficients h_n are real or complex numbers.

Suppose that the scaling function $\phi(x)$ is compactly supported. Then only finitely many of the coefficients, say $h_0, h_1, \ldots, h_N$, are nonzero, and $\phi(x)$ is supported on the interval $[0,N]$. Note that then (8.3) is a special case ($\alpha = 2$) of (5.10) discussed in Section 5.2. Because of Theorem 5.5.4, it makes sense to assume that $\sum h_n = 2$.

In this case, a *wavelet* $\psi(x)$ associated with the multiresolution analysis can be generated by the formula

$$\psi(x) = \sum_{k\in\mathbb{Z}} (-1)^k h_{N-k} \phi(2x-k). \tag{8.4}$$

The wavelet $\psi(x)$ is also supported on the interval $[0,N]$. Both $\phi(x)$ and $\psi(x)$ depend only on the sequence of coefficients $h_0, h_1, \ldots, h_N$. Compactly supported scaling functions and wavelets can thus be generated by starting from a suitable sequence of coefficients. In fact, the first example of a compactly supported wavelet was constructed by Daubechies in just this manner. See [111] for more information about this construction, or about wavelets and multiresolution analysis in general.

These scaling functions and wavelets may not have a closed form representation. In practice, this is not a problem, since it is the sequence of coefficients that are used in applications, rather than the scaling function or wavelet themselves. Indeed, the Fourier transform of the sequence of coefficients

$$m(\xi) = \sum_n h_n e^{-2\pi i n \xi}$$

is called the *low-pass filter* for the scaling function $\phi(x)$, and is an important tool in studying multiresolution analyses and wavelets.We may wish to visualize the scaling function $\phi(x)$ or wavelet $\psi(x)$, however. This can be done as follows using a chaos game.

We first vectorize the scaling equation, as follows: Define $V_\phi : [0,1] \to \mathbb{R}$ by

$$V_\phi(x) = \begin{bmatrix} \phi(x) \\ \phi(x+1) \\ \vdots \\ \phi(x+N-1) \end{bmatrix}.$$

Define matrices T_0 and T_1 by

$$(T_0)_{i,j} = h_{2i-j-1},$$
$$(T_1)_{i,j} = h_{2i-j}.$$

Let $\tau : [0,1] \to [0,1]$ be the mapping $\tau(x) = 2x \pmod 1$. Then, the scaling equation can be written

$$V_\phi(x) = T_\omega V_\phi(\tau x), \tag{8.5}$$

where ω is the first digit of the binary expansion of x. That is, $2x = \omega + \tau x$.

The chaos game in this example will update the values of both x and $V_\phi(x)$ in each iteration. To update x, we will use the mappings $w_0, w_1 : [0,1] \to [0,1]$ defined by

$$w_0(x) = \frac{x}{2},$$
$$w_1(x) = \frac{x}{2} + \frac{1}{2}.$$

To update $V_\phi(x)$, we will use the mappings T_0 and T_1 defined above. To initialize the chaos game, we set $x_0 = 0$ and set $V_{\phi,0}$ to be a fixed point of the map T_0 (that is, $V_{\phi,0}$ is a specific vector

$$V_{\phi,0} = \begin{bmatrix} v_{0,0} \\ v_{1,0} \\ \vdots \\ v_{N,0} \end{bmatrix},$$

where we will set $\phi(x_0) := v_{0,0}$, $\phi(x_0+1) := v_{1,0}$, and so on up to $\phi(x_0+N-1) := v_{N,0}$).

For each iteration of the chaos game, we choose $\alpha_n = 0,1$ uniformly and update

$$x_n = w_{\alpha_n}(x_{n-1}),$$

$$V_{\phi,n} = \begin{bmatrix} v_{0,n} \\ v_{1,n} \\ \vdots \\ v_{N,n} \end{bmatrix} = T_{\alpha_n} V_{\phi,n-1}.$$

We set $V_\phi(x_n)$ to be equal to $V_{\phi,n}$, so that $\phi(x_n) = v_{0,n}$, $\phi(x_n+1) = v_{1,n}$, and so on to $\phi(x_n+N-1) = v_{N,n}$. Then, we plot the points $(x_n, \phi(x_n))$, $(x_n+1, \phi(x_n+1))$, through $(x_n+N-1, \phi(x_n+N-1))$.

The wavelet $\psi(x)$ can be visualized similarly. We may vectorize (8.4) by forming the vector

$$V_\psi(x) = \begin{bmatrix} \psi(x) \\ \psi(x+1) \\ \vdots \\ \psi(x+N-1) \end{bmatrix}$$

and defining mappings H_0 and H_1 by

$$(H_0)_{i,j} = (-1)^k h_{N-k},\ k = 2i-j-1,$$
$$(H_1)_{i,j} = (-1)^{k'} h_{N-k'},\ k' = 2i-j.$$

We then use V_ψ, H_0, and H_1 in place of V_ϕ, T_0, and T_1, respectively, in the chaos game described above.

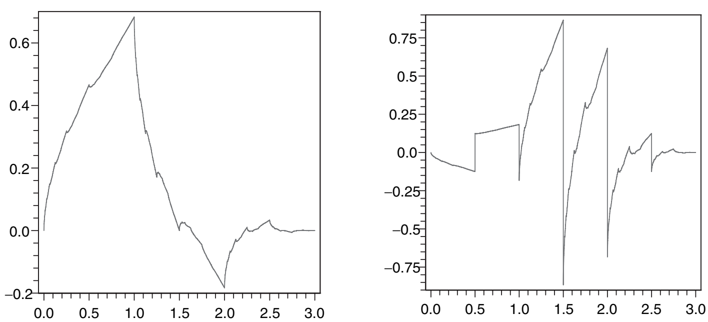


Figure 8.9. Chaos game for the Daubechies' D_3 wavelet (L) and scaling function (R) after 1000 iterations.

Several iterations of this algorithm for the Daubechies' D_3 wavelet, one of the first examples of a compactly supported wavelet, are shown in Figure 8.9. The Daubechies' D_3 wavelet is supported on the interval $[0,3]$ and has coefficients $h_0 = \frac{1+\sqrt{3}}{4}$, $h_1 = \frac{3+\sqrt{3}}{4}$, $h_2 = \frac{3-\sqrt{3}}{4}$, and $h_3 = \frac{1-\sqrt{3}}{4}$ [110]. ◇

8.5.2 More on Visualizing DNA

In the opening example, we used a deterministic sequence of DNA bases to update a point x_n in the attractor of an iterated function system, rather than randomly choosing with which of the four vertices of the square to average the previous point x_{n-1}. If we instead choose the base ω_n randomly, then we have a true chaos game.

Let $p_{\beta,k}(seq)$ be the probability that base β (β = A, C, G, or T) follows the subsequence *seq* of length k. Thus, $p_{\mathrm{A},1}(\mathrm{T})$ is the probability that $x_n = \mathrm{A}$ given that $x_{n-1} = \mathrm{T}$, while $p_{\mathrm{A},2}(\mathrm{GG})$ is the probability that $x_n = \mathrm{A}$ given that $x_{n-1} = \mathrm{G}$ and that $x_{n-2} = \mathrm{G}$. If the nth base is selected uniformly at random, with no dependence on the preceding sequence, then we do not get a very interesting picture out of the chaos game. However, in most organisms, these probabilities are not uniformly distributed. As well, the probabilities $p_{\beta,k}(seq)$ vary by organism. Ashlock and Golden [8] have shown that different organisms yield distinct chaos games (see Figure 8.10).

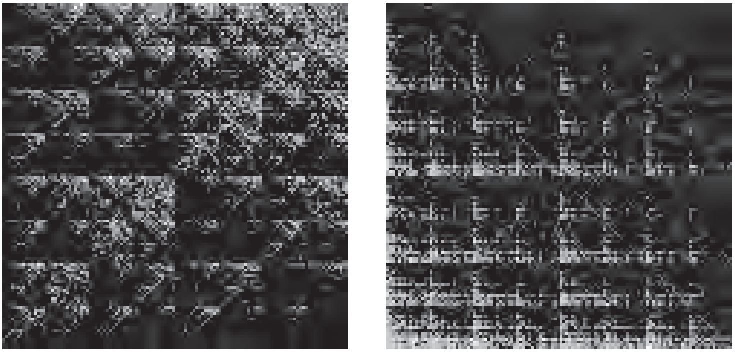


Figure 8.10. Chaos games for mycobacterium tuberculosis (L) and human chromosome 22 (R); the darker the shade, the higher the frequency of "hits."

8.6 Hilbert's Inequality and Witten's Zeta Function

We next explore a variety of pleasing connections between analysis, number theory, and operator theory, while exposing a number of beautiful inequalities originating with Hilbert. We shall first establish the afore-mentioned inequality [160, 260] and then apply it to various multiple zeta values. In consequence we obtain the norm of Hilbert's matrix.

8.6.1 Hilbert's (Easier) Inequality

A useful preparatory lemma is the following:

Lemma 8.6. *For* $0 < a < 1$ *and* $n = 1, 2, \ldots$,

$$\sum_{m=1}^{\infty} \frac{1}{(n+m)(m/n)^a} < \int_0^{\infty} \frac{1}{(1+x)x^a}\,dx < \frac{(1/n)^{1-a}}{1-a} + \sum_{m=1}^{\infty} \frac{1}{(n+m)(m/n)^a},$$

and

$$\int_0^{\infty} \frac{1}{(1+x)x^a}\,dx = \pi \csc(a\pi).$$

Proof: The inequalities come from using standard rectangular approximations to a monotonic integrand and overestimating the integral from 0 to $1/n$. □

The evaluation of the integral is in various tables and is known to *Maple* or *Mathematica*. We offer two other proofs:
Proof:

(i) Write

$$\begin{aligned}
\int_0^{\infty} \frac{1}{(1+x)x^a}\,dx &= \int_0^1 \frac{x^{-a}+x^{a-1}}{1+x}\,dx \\
&= \sum_{n=0}^{\infty} (-1)^n \left\{ \frac{1}{n+1-a} + \frac{1}{n+a} \right\} \\
&= \sum_{n=1}^{\infty} (-1)^n \left\{ \frac{1}{n+a} - \frac{1}{n-a} \right\} + \frac{1}{a} \\
&= \frac{1}{a} - \sum_{n=1}^{\infty} \frac{(-1)^n\, 2a}{a^2-n^2} = \pi \csc(a\pi),
\end{aligned}$$

since the last equality is the classical partial fraction identity for $\pi\csc(a\pi)$.

(ii) Alternatively, we begin by letting $1+x = 1/y$,

$$\begin{aligned}
\int_0^{\infty} \frac{x^{-a}}{1+x}\,dx &= \int_0^1 y^{a-1}(1-y)^{-a}\,dy \\
&= B(a, 1-a) = \Gamma(a)\,\Gamma(1-a) = \frac{\pi}{\sin(a\pi)}.
\end{aligned}$$

□

Combining the arguments in (i) and (ii) above actually derives the Gamma function's reflection formula (7.7), i.e.,

$$\Gamma(a)\,\Gamma(1-a) = \frac{\pi}{\sin(a\pi)},$$

from the partial fraction for cosec or vice versa—especially if we appeal to the Bohr-Mollerup theorem to establish $B(a,1-a) = \Gamma(a)\,\Gamma(1-a)$.

Theorem 8.7 (Hilbert Inequality). *For nonnegative sequences (a_n) and (b_n), not both zero, and for $1 \le p,q \le \infty$ with $1/p + 1/q = 1$ one has*

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{a_n\, b_m}{n+m} < \pi \csc\left(\frac{\pi}{p}\right) \|a_n\|_p\, \|b_n\|_q. \tag{8.6}$$

Proof: Fix $\lambda > 0$. We apply Hölder's inequality with "compensating difficulties" to obtain

$$\begin{aligned}
\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{a_n\, b_m}{n+m} &= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{a_n}{(n+m)^{1/p}(m/n)^{\lambda/p}} \frac{b_m}{(n+m)^{1/q}(n/m)^{\lambda/p}} \\
&\le \left(\sum_{n=1}^{\infty} |a_n|^p \sum_{m=1}^{\infty} \frac{1}{(n+m)(m/n)^{\lambda}}\right)^{1/p} \\
&\quad \times \left(\sum_{m=1}^{\infty} |b_m|^q \sum_{n=1}^{\infty} \frac{1}{(n+m)(n/m)^{\lambda q/p}}\right)^{1/q} \\
&< \pi\, |\csc(\pi\lambda)|^{1/p}\, |\csc((q-1)\pi\lambda)|^{1/q}\, \|a_n\|_p\, \|b_m\|_q,
\end{aligned} \tag{8.7}$$

so that the left-hand side of (8.6) is no greater than $\pi \csc\left(\frac{\pi}{p}\right) \|a_n\|_p\, \|b_n\|_q$ on setting $\lambda = 1/q$ and appealing to symmetry in p,q. □

The integral analogue of Theorem 8.7 may likewise be established. There are numerous extensions. One of interest for us later is

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{a_n\, b_m}{(n+m)^{\tau}} < \left\{\pi \csc\left(\frac{\pi(q-1)}{\tau q}\right)\right\}^{\tau} \|a_n\|_p\, \|b_n\|_q, \tag{8.8}$$

valid for $p,q > 1, \tau > 0, 1/p + 1/q \ge 1$, and $\tau + 1/p + 1/q = 2$. The best constant $C(p,q,\tau) \le \{\pi \csc(\pi(q-1)/(\tau q))\}^{\tau}$ is called the *Hilbert constant* [136, §3.4].

For $p = 2$, Theorem 8.7 becomes Hilbert's original inequality:

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{a_n\,b_m}{n+m} \le \pi\sqrt{\sum_{n=1}^{\infty}|a_n|^2}\sqrt{\sum_{n=1}^{\infty}|b_n|^2}, \tag{8.9}$$

though Hilbert only obtained the constant 2π [159].

A fine direct Fourier analytic proof starts from the observation that

$$\frac{1}{2\pi i}\int_0^{2\pi}(\pi - t)\,e^{int}\,dt = \frac{1}{n},$$

for $n = 1, 2\ldots$, and deduces

$$\sum_{n=1}^{N}\sum_{m=1}^{N}\frac{a_n\,b_m}{n+m} = \frac{1}{2\pi i}\int_0^{2\pi}(\pi - t)\sum_{k=1}^{N}a_k\,e^{ikt}\sum_{k=1}^{N}b_k\,e^{ikt}\,dt. \tag{8.10}$$

We recover (8.9) by applying the integral form of the Cauchy-Schwarz inequality to the integral side of the representation (8.10).

Likewise,

$$\sum_{n=1}^{N}\sum_{m=1}^{N}\frac{a_n\,b_m}{(n+m)^2} = \frac{1}{2\pi}\int_0^{2\pi}\left(\zeta(2) - \frac{\pi t}{2} + \frac{1}{4}\right)\sum_{k=1}^{N}a_k\,e^{ikt}\sum_{k=1}^{N}b_k\,e^{ikt}\,dt,$$

and more generally

$$\sum_{n=1}^{N}\sum_{m=1}^{N}\frac{a_n\,b_m}{(n+m)^\sigma} = \frac{1}{2\pi i^\sigma}\int_0^{2\pi}\psi_\sigma\left(\frac{t}{2\pi}\right)\sum_{k=1}^{N}a_k\,e^{ikt}\sum_{k=1}^{N}b_k\,e^{ikt}\,dt,$$

since

$$\psi_{2n}(x) = \sum_{k=1}^{\infty}\frac{\cos(2k\pi x)}{k^{2n}}, \qquad \psi_{2n+1}(x) = \sum_{k=1}^{\infty}\frac{\sin(2k\pi x)}{k^{2n+1}},$$

where $\psi_\sigma(x)$ are related to the *Bernoulli polynomials* by

$$\psi_\sigma(x) = (-1)^{\lfloor(1+\sigma)/2\rfloor}\,B_\sigma(x)\,\frac{(2\pi)^\sigma}{2\,\sigma!},$$

for $0 < x < 1$. It follows that

$$\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{a_n\,b_m}{(n+m)^\sigma} \le \|\psi_\sigma\|_{[0,1]}\,\|a\|_2\,\|b\|_2,$$

where for $n > 0$ we compute

$$\|\psi_{2n}\|_{[0,1]} = \psi_{2n}(0) = \zeta(2n) \quad \text{and} \quad \|\psi_{2n+1}\|_{[0,1]} = \psi_{2n+1}(1/4) = \beta(2n+1),$$

where we use $\beta(n) := \sum_{k=0}^{\infty}(-1)^k \frac{1}{(2k+1)^n}$.

This and much more of the early twentieth-century history—and philosophy—of the *"'bright' and amusing"* subject of inequalities is charmingly discussed in Hardy's retirement lecture as London Mathematical Society Secretary [159]. He comments [159, p. 474] that "Harald Bohr is reported to have remarked 'Most analysts spend half their time hunting through the literature for inequalities they want to use, but cannot prove.'"

This remains true, though more recent inequalities often involve less linear objects such as entropies, divergences, and log-barrier functions [50, 70], such as the *divergence estimate* [68, p. 63]

$$\sum_{n=1}^{N} p_i \log\left(\frac{p_i}{q_i}\right) \geq \frac{1}{2}\left(\sum_{n=1}^{N} |p_i - q_i|\right)^2,$$

valid for any two strictly positive sequences with $\sum_{i=1}^{N} p_i = \sum_{i=1}^{N} q_i = 1$.

Two other high spots in Hardy's essay are *Carleman's inequality*

$$\sum_{n=1}^{\infty} (a_1\, a_2 \cdots a_n)^{1/n} \leq e \sum_{n=1}^{\infty} a_n$$

(see also [51, p. 284]) and Hardy's own

$$\sum_{n=1}^{\infty} \left(\frac{a_1 + a_2 + \cdots + a_n}{n}\right)^p \leq \left(\frac{p}{p-1}\right)^p \sum_{n=1}^{\infty} a_n^p, \tag{8.11}$$

for $p > 1$. Hardy comments [159, p. 485] that his "own theorem was discovered as a by-product of my own attempt to find a really simple and elementary proof of Hilbert's." For $p = 2$, Hardy reproduces Elliott's proof of (8.11), writing "it can hardly be possible to find a proof more concise or elegant." It is as follows. Set $A_n := a_1 + a_2 + \cdots + a_n$, and write

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

something easy to check symbolically, and sum to obtain

$$\sum_n \left(\frac{A_n}{n}\right)^2 \leq 2\sum_n \frac{a_n A_n}{n} \leq 2\sqrt{\sum_n a_n^2}\sqrt{\sum_n \left(\frac{A_n}{n}\right)^2},$$

which proves (8.11) for $p = 2$. This easily adapts to the general case.

Finally we record the (harder) *Hilbert inequality* as

$$\left| \sum_{n \neq m \in \mathbf{Z}} \frac{a_n\, b_m}{n-m} \right| < \pi \sqrt{\sum_{n=1}^{\infty} |a_n|^2} \sqrt{\sum_{n=1}^{\infty} |b_n|^2}, \tag{8.12}$$

the best constant π being due to Schur in 1911 [216]. There are many extensions—with applications to prime number theory [216].

8.6.2 Witten ζ-functions

Let us recall that initially for $r, s > 1/2$,

$$\mathscr{W}(r,s,t) := \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{n^r\, m^s\, (n+m)^t}$$

is a *Witten ζ-function* [106, 131, 287]. We refer to [287] for a description of the uses of more general Witten ζ-functions. Ours are also—more accurately—called *Tornheim double sums* or *Tornheim-Zagier sums*, see [131] and Section 7.9. Correspondingly,

$$\zeta(t,s) := \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{m^s\, (n+m)^t} = \sum_{n>m>0} \frac{1}{n^t\, m^s}$$

is an *Euler double sum* of the sort met in Chapters 1 and 2.

Example 8.8. Let $a_n := 1/n^r$, $b_n := 1/n^s$. Then the inequality (8.9) becomes

$$\mathscr{W}(r,s,1) \leq \pi \sqrt{\zeta(2r)} \sqrt{\zeta(2s)}. \tag{8.13}$$

Similarly, the inequality (8.6) becomes

$$\mathscr{W}(r,s,1) \leq \pi \csc\left(\frac{\pi}{p}\right) \sqrt[p]{\zeta(pr)} \sqrt[q]{\zeta(qs)}. \tag{8.14}$$

Indeed, (8.8) can be used to estimate $\mathscr{W}(r,s,\tau)$ for somewhat broader $\tau \neq 1$. ◇

There is a simple algebraic relation

$$\mathscr{W}(r,s,t) = \mathscr{W}(r-1,s,t+1) + \mathscr{W}(r,s-1,t+1). \tag{8.15}$$

This is based on writing

$$\frac{m+n}{(m+n)^{t+1}} = \frac{m}{(m+n)^{t+1}} + \frac{n}{(m+n)^{t+1}}.$$

Also

$$\mathscr{W}(r,s,t) = \mathscr{W}(s,r,t), \tag{8.16}$$

and

$$\mathscr{W}(r,s,0) = \zeta(r)\,\zeta(s) \quad \text{while} \quad \mathscr{W}(r,0,t) = \zeta(t,r). \tag{8.17}$$

Hence, $\mathscr{W}(s,s,t) = 2\mathscr{W}(s,s-1,t+1)$, and so

$$\mathscr{W}(1,1,1) = 2\mathscr{W}(1,0,2) = 2\,\zeta(2,1) = 2\,\zeta(3). \tag{8.18}$$

In particular, (8.18) implies that $\zeta(3) \le \pi^3/12$, on appealing to (8.13) above. For many proofs of this basic identity $\zeta(2,1) = \zeta(3)$, we refer to [60]. We note that the analogue to (8.15), $\zeta(s,t)+\zeta(t,s) = \zeta(s)\,\zeta(t) - \zeta(s+t)$, shows that $\mathscr{W}(s,0,s) = 2\,\zeta(s,s) = \zeta^2(s) - \zeta(2s)$. In particular, $\mathscr{W}(2,0,2) = 2\,\zeta(2,2) = \pi^4/36 - \pi^4/90 = \pi^4/72$.

More generally, recursive use of (8.15) and (8.16), along with initial conditions (8.17), shows that all integer $\mathscr{W}(s,r,t)$ values are expressible in terms of double (and single) Euler sums. As we shall see in (8.23), the representations are necessarily homogeneous polynomials of *weight* $r+s+t$. All double sums of weight less than 8 and all those of odd weight reduce to sums of products of single variable zeta values [51]. The first impediments are because $\zeta(6,2)$ and $\zeta(5,3)$ are not reducible.

We also observe that, in terms of the polylogarithm function $\mathrm{Li}_s(t) = \sum_{n>0} t^n/n^s$ for real s, the representation (8.10) yields

$$\mathscr{W}(r,s,1) = \frac{1}{2\pi i}\int_{-\pi}^{\pi} \sigma\,\mathrm{Li}_r(-e^{-i\sigma})\,\mathrm{Li}_s(-e^{-i\sigma})\,d\sigma. \tag{8.19}$$

This representation is not numerically effective. It is better to start with

$$\Gamma(t)/(m+n)^t = \int_0^1 (-\log\sigma)^{t-1}\,\sigma^{m+n-1}\,d\sigma$$

and so to obtain

$$\mathscr{W}(r,s,t) = \frac{1}{\Gamma(t)}\int_0^1 \mathrm{Li}_r(\sigma)\,\mathrm{Li}_s(\sigma)\,\frac{(-\log\sigma)^{t-1}}{\sigma}\,d\sigma. \tag{8.20}$$

This real variable analogue of (8.19) is much more satisfactory computationally. For example, we recover an analytic proof of

$$2\,\zeta(2,1) = \mathscr{W}(1,1,1) = \int_0^1 \frac{\log^2(1-\sigma)}{\sigma}\,d\sigma = 2\,\zeta(3). \tag{8.21}$$

Moreover, we may now discover analytic as opposed to algebraic relations. Integration by parts yields

$$\mathscr{W}(r,s+1,1)+\mathscr{W}(r+1,s,1)=\mathrm{Li}_{r+1}(1)\,\mathrm{Li}_{s+1}(1)=\zeta(r+1)\,\zeta(s+1). \tag{8.22}$$

So, in particular, $\mathscr{W}(s+1,s,1)=\zeta^2(s+1)/2$.

Symbolically, *Maple* immediately evaluates $\mathscr{W}(2,1,1)=\pi^4/72$, and while it fails directly with $\mathscr{W}(1,1,2)$, we know it must be a multiple of π^4 or equivalently $\zeta(4)$; numerically we obtain

$$\mathscr{W}(1,1,2)/\zeta(4)=.49999999999999999998\ldots.$$

Continuing, for $r+s+t=5$ the only terms to consider are $\zeta(5)$ and $\zeta(2)\zeta(3)$, and *PSLQ* yields the following weight-five relations:

$$\begin{aligned}
\mathscr{W}(2,2,1) &= \int_0^1 \frac{\mathrm{Li}_2(x)^2}{x}\,dx = 2\,\zeta(3)\,\zeta(2)-3\,\zeta(5),\\
\mathscr{W}(2,1,2) &= \int_0^1 \frac{\mathrm{Li}_2(x)\log(1-x)\log(x)}{x}\,dx = \zeta(3)\,\zeta(2)-\frac{3}{2}\,\zeta(5),\\
\mathscr{W}(1,1,3) &= \int_0^1 \frac{\log^2(x)\log^2(1-x)}{2x}\,dx = -2\,\zeta(3)\,\zeta(2)+4\,\zeta(5),\\
\mathscr{W}(3,1,1) &= \int_0^1 \frac{\mathrm{Li}_3(x)\log(1-x)}{x}\,dx = \zeta(3)\,\zeta(2)+3\,\zeta(5),
\end{aligned}$$

as predicted.

Likewise, for $r+s+t=6$ the only terms we need to consider are $\zeta(6)$ and $\zeta^2(3)$ since $\zeta(6),\zeta(4)\,\zeta(2)$, and $\zeta^3(2)$ are all rational multiples of π^6. We recover identities like

$$\mathscr{W}(3,2,1)=\int_0^1 \frac{\mathrm{Li}_3(x)\,\mathrm{Li}_2(x)}{x}\,dx=\frac{1}{2}\,\zeta^2(3),$$

consistent with (8.22) below.

The general form of the reduction, for integers r,s, and t, is due to Tornheim and expresses $\mathscr{W}(r,s,t)$ in terms of $\zeta(a,b)$ with weight $a+b=N:=r+s+t$ [131]:

$$\mathscr{W}(r,s,t)=\sum_{i=1}^{r\vee s}\left\{\binom{r+s-i-1}{s-1}+\binom{r+s-i-1}{r-1}\right\}\zeta(i,N-i). \tag{8.23}$$

Various other general formulas are given in [131] for classes of sums such as $\mathscr{W}(2n+1,2n+1,2n+1)$ and $\mathscr{W}(2n,2n,2n)$.

8.6.3 The Best Constant

It turns out that the constant π used in Theorem 8.7 is best possible [160].

Example 8.9. Let us numerically explore the ratio

$$\mathscr{R}(s) := \frac{\mathscr{W}(s,s,1)}{\pi\,\zeta(2s)}$$

as $s \to 1/2^+$. Remember that $\mathscr{R}(1) = 12\,\zeta(3)/\pi^3 \approx 0.4652181552\ldots$.

Initially, we may directly sum as follows:

$$\begin{aligned}
\mathscr{W}(s,s,1) &= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{m^{-s}n^{-s}}{m+n} \\
&= 2\sum_{n=1}^{\infty}\frac{1}{n^{2s}}\sum_{m=1}^{n-1}\frac{1/n}{(m/n)^s(m/n+1)} + \frac{\zeta(2s+1)}{2} \\
&\le 2\,\zeta(2s)\int_0^1 \frac{x^{-s}}{1+x}\,dx + \frac{\zeta(2s+1)}{2} \\
&\le 2\sum_{n=1}^{\infty}\frac{1}{n^{2s}}\sum_{m=1}^{n}\frac{1/n}{(m/n)^s(m/n+1)} + \frac{\zeta(2s+1)}{2} \\
&= 2\sum_{n=1}^{\infty}\frac{1}{n^{2s}}\sum_{m=1}^{n-1}\frac{1/n}{(m/n)^s(m/n+1)} + \frac{3\zeta(2s+1)}{2} \\
&= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{m^{-s}n^{-s}}{m+n} + \zeta(2s+1).
\end{aligned}$$

We deduce that $\mathscr{R}(s) \sim \mathscr{I}(s) := 2/\pi \int_0^1 x^{-s}/(1+x)\,dx$ as $s \to 1/2$. Since Lemma 8.6 and the substitution $x \mapsto 1/x$ imply $\mathscr{I}\left(\frac{1}{2}\right) = 1$, we get $\lim_{s\to 1/2}\mathscr{R}(s) = 1$. ◇

Further numerical explorations seem in order, which will lead us to a more visual understanding and then a direct proof of this relation. For $1/2 < s < 1$, (8.20) is hard to use numerically and led us to look for a more sophisticated attack along the line of the Hurwitz zeta function and Bernoulli polynomial integrals used in [131], or more probably the expansions in [106]. Namely,

$$\mathscr{W}(r,s,t) = \int_0^1 E(r,x)\,E(s,x)\,\overline{E(t,x)}\,dx, \tag{8.24}$$

where $E(s,x) := \sum_{n=1}^{\infty} e^{2\pi i n x}\,n^{-s} = \mathrm{Li}_s\left(e^{2\pi i x}\right)$, using the formulas

$$E(s,x) = \sum_{m=0}^{\infty}\zeta(s-m)\,\frac{(2\pi i x)^m}{m!} + \Gamma(1-s)\,(-2\pi i x)^{s-1},$$

for $|x| < 1$ and

$$E(s,x) = -\sum_{m=0}^{\infty} \eta(s-m) \frac{(2x-1)^m (\pi i)^m}{m!},$$

with $\eta(s) := (1-2^{1-s})\zeta(s)$, for $0 < x < 1$ as given in [106, (2.6) and (2.9)].

Indeed, carefully expanding (8.24) with a free parameter $\theta \in (0,1)$ leads to the following efficient formula *when neither r nor s is an integer:*

$$\begin{aligned}\Gamma(t)\mathscr{W}(r,s,t) = &\sum_{m,n\geq 1} \frac{\Gamma(t,(m+n)\theta)}{m^r n^s (m+n)^t} \\ &+ \sum_{u,v\geq 0} (-1)^{u+v} \frac{\zeta(r-u)\zeta(s-v)\theta^{u+v+t}}{u!v!(u+v+t)} \\ &+ \Gamma(1-r) \sum_{v\geq 0} (-1)^v \frac{\zeta(s-v)\theta^{r+v+t-1}}{v!(r+v+t-1)} \\ &+ \Gamma(1-s) \sum_{u\geq 0} (-1)^u \frac{\zeta(r-u)\theta^{s+u+t-1}}{u!(s+u+t-1)} \\ &+ \Gamma(1-r)\Gamma(1-s) \frac{\theta^{r+s+t-2}}{r+s+t-2},\end{aligned} \tag{8.25}$$

where $\Gamma(t,z)$ is the incomplete gamma function

$$\Gamma(t,z) := \int_z^{\infty} x^{t-1} e^{-x}\, dx. \tag{8.26}$$

When one or both of r and s is an integer, a limit formula with a few more terms results. We can now accurately plot $\mathscr{R}$ and $\mathscr{I}$ on $[1/3, 2/3]$, as shown in Figure 8.11, and so again see $\lim_{s\to 1/2} \mathscr{R}(s) = 1$.

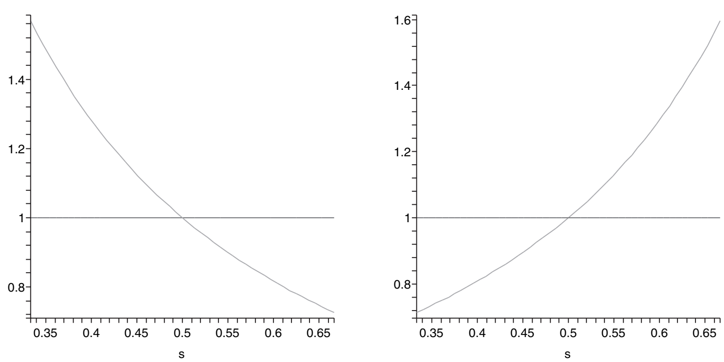


Figure 8.11. $\mathscr{R}$ (left) and $\mathscr{I}$ (right) on $[1/3, 2/3]$.

Proof of the limit: To establish this directly, we denote

$$\sigma_n(s) := \sum_{m=1}^{\infty} n^s m^{-s}/(n+m)$$

and appeal to Lemma 8.6 to write

$$\begin{aligned}
\mathscr{L} : &= \lim_{s\to 1/2}(2s-1)\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{n^{-s}m^{-s}}{n+m} \\
&= \lim_{s\to 1/2}(2s-1)\sum_{n=1}^{\infty}\frac{1}{n^{2s}}\,\sigma_n(s) \\
&= \lim_{s\to 1/2}(2s-1)\sum_{n=1}^{\infty}\frac{\{\sigma_n(s)-\pi\csc(\pi s)\}}{n^{2s}} \\
&\quad + \lim_{s\to 1/2}\frac{\pi\,(2s-1)\zeta(2s)}{\sin\pi s} \\
&= 0+\pi,
\end{aligned}$$

since, by another appeal to Lemma 8.6, the parenthetic term is $O(n^{s-1})$ while in the second $\zeta(2s) \sim 1/(2s-1)$ as $s \to 1/2^+$. □

In consequence, we see that $\mathscr{L} = \lim_{s\to 1/2}\mathscr{R}(s) = 1$, and—at least to first-order—inequality (8.9) is best possible; see also [172].

Likewise, the constant in Theorem 8.7 is the best possible. Motivated by the above argument, we consider

$$\mathscr{R}_p(s) := \frac{\mathscr{W}((p-1)s,s,1)}{\pi\,\zeta(ps)}$$

and observe that, with $\sigma_n^p(s) := \sum_{m=1}^{\infty}(n/m)^{-(p-1)s}/(n+m) \to \pi\csc\left(\frac{\pi}{q}\right)$, we have

$$\begin{aligned}
\mathscr{L}_p : &= \lim_{s\to 1/p}(ps-1)\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{n^{-s}m^{-(p-1)s}}{n+m} \\
&= \lim_{s\to 1/p}(ps-1)\sum_{n=1}^{\infty}\frac{1}{n^{ps}}\,\sigma_n^p(s) \\
&= \lim_{s\to 1/p}(ps-1)\sum_{n=1}^{\infty}\frac{\left\{\sigma_n^p(s)-\pi\csc(\pi/q))\right\}}{n^{ps}} \\
&\quad + \lim_{s\to 1/p}(2s-1)\zeta(ps)\,\pi\csc\left(\frac{\pi}{q}\right) \\
&= 0+\pi\csc\left(\frac{\pi}{q}\right).
\end{aligned}$$

Setting $r := (p-1)s, s \to 1/p^+$, we check that $\zeta(ps)^{1/p}\zeta(qr)^{1/q} = \zeta(ps)$, and hence the best constant in (8.14) is the one given. To recapitulate in terms of the celebrated infinite *Hilbert matrices,* $\mathscr{H}_0 := \{1/(m+n)\}_{m,n=1}^{\infty}$ and $\mathscr{H}_1 := \{1/(m+n-1)\}_{m,n=1}^{\infty}$, [51, pp. 250–252], we have actually proven

Theorem 8.10. *Let $1 < p, q < \infty$ be given with $1/p + 1/q = 1$. The Hilbert matrices $\mathscr{H}_0$ and $\mathscr{H}_1$ determine bounded linear mappings from the sequence space ℓ^p to itself such that*

$$\|\mathscr{H}_1\|_{p,p} = \|\mathscr{H}_0\|_{p,p} = \lim_{s \to 1/p} \frac{\mathscr{W}(s,(p-1)s,1)}{\zeta(ps)} = \pi \csc\left(\frac{\pi}{p}\right).$$

Proof: Appealing to the isometry between $(\ell^p)^*$ and ℓ^q, and given the evaluation $\mathscr{L}_p$ above, we directly compute the operator norm of $\mathscr{H}_0$ as

$$\|\mathscr{H}_0\|_{p,p} = \sup_{\|x\|_p=1} \|\mathscr{H}_0 x\|_p = \sup_{\|y\|_q=1} \sup_{\|x\|_p=1} \langle \mathscr{H}_0 x, y\rangle = \pi \csc\left(\frac{\pi}{p}\right).$$

Now clearly $\|\mathscr{H}_0\|_{p,p} \le \|\mathscr{H}_1\|_{p,p}$. For $n \ge 2$ we have

$$\sum_{m=1}^{\infty} \frac{1}{(n+m-1)(m/n)^a} \le \sum_{m=1}^{\infty} \frac{1}{(n-1+m)(m/(n-1))^a} \le \pi \csc(\pi a),$$

and an appeal to Lemma 8.6 and Theorem 8.7 shows that $\|\mathscr{H}_0\|_{p,p} \ge \|\mathscr{H}_1\|_{p,p}$. □

A delightful operator-theoretic introduction to the Hilbert matrix $\mathscr{H}_0$ is given by Choi in his Chauvenet prize winning article [89] while a recent set of notes by G. J. O. Jameson [172] is also well worth accessing.

In the case of (8.8), Finch [136, §4.3] comments that the issue of best constants is unclear in the literature. He remarks that even the case $p = q = 4/3, \tau = 1/2$ appears to be open. It seems improbable that the techniques of this note can be used to resolve the question. Indeed, consider $\mathscr{R}_{1/2}(s,\alpha) : \mathscr{W}(s,s,1/2)/\zeta(4s/3)^{\alpha}$, with the critical point in this case being $s = 3/4$.

Numerically, using (8.25) we discover that

$$\log(\mathscr{W}(s,s,1/2))/\log(\zeta(4s/3)) \to 0.$$

Hence, for any $\alpha > 0$, the requisite limit, $\lim_{s\to 3/4} \mathscr{R}_{1/2}(s,\alpha) = 0$, which is certainly not the desired norm. What we are exhibiting is that the subset of sequences $(a_n) = (n^{-s})$ for $s > 0$ is *norming* in ℓ^p for $\tau = 1$ but not apparently for general $\tau > 0$.

One may also study the corresponding behavior of Hardy's inequality (8.11). For example, setting $a_n := 1/n$ and denoting $H_n := \sum_{k=1}^{n} 1/k$ in (8.11) yields

$$\sum_{n=1}^{\infty} \left(\frac{H_n}{n}\right)^p \leq \left(\frac{p}{p-1}\right)^p \zeta(p).$$

Application of the integral test and the evaluation

$$\int_1^{\infty} \left(\frac{\log x}{x}\right)^p dx = \frac{\Gamma(1+p)}{(p-1)^{p+1}},$$

for $p > 1$ easily shows that the constant is again best possible.

8.7 Computational Challenge Problems

In [50] we gave ten challenge problems and indicated that the solutions could be found scattered through [50] and [51]. Subsequently, an annotated and much enhanced version of the promised solutions has been published in the *American Mathematical Monthly* [21]. Our set was triggered by Nick Trefethen's *SIAM 100 Digit Challenge*, wonderfully described in [275] and reviewed in [48]. We conclude this chapter with a visit to two of the high spots of our problem set.

8.7.1 Finding $\zeta(3,1,3,1)$

Problem 9. *Calculate*

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

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

History and context. In the notation introduced before (in Section 2.4.4), we ask for the value of $\zeta(3,1,3,1)$. The study of such sums in two variables, as we noted, originates with Euler. These investigations were apparently due to a serendipitous mistake. Goldbach wrote to Euler [50, pp. 99–100]:

> When I recently considered further the indicated sums of the last two series in my previous letter, I realized immediately that the same series arose due to a mere writing error, from which indeed the saying goes, "Had one not erred, one would have achieved less. [*Si non errasset, fecerat ille minus*.]"

Euler's *reduction formula* is

$$\zeta(s,1) \quad = \quad \frac{s}{2}\zeta(s+1) - \frac{1}{2}\sum_{k=1}^{s-2}\zeta(k+1)\zeta(s+1-k),$$

which *reduces* the given double Euler sums to a sum of products of classical ζ-values. Euler also noted the first *reflection formula*

$$\zeta(a,b)+\zeta(b,a) \quad = \quad \zeta(a)\zeta(b)-\zeta(a+b),$$

certainly valid when $a > 1$ and $b > 1$. This is an easy algebraic consequence of adding the double sums. Another marvelous fact is the *sum formula*

$$\sum_{\Sigma a_i = n, a_i \geq 0} \zeta\left(a_1+2, a_2+1, \cdots, a_r+1\right) \quad = \quad \zeta(n+r+1) \tag{8.27}$$

for nonnegative integers n and r. This, as David Bradley observes, is equivalent to the generating function identity

$$\sum_{n>0} \frac{1}{n^r(n-x)} \quad = \quad \sum_{k_1>k_2>\cdots k_r>0} \prod_{j=1}^{r} \frac{1}{k_j - x}.$$

The first three nontrivial cases of (8.27) are $\zeta(3) = \zeta(2,1), \zeta(4) = \zeta(3,1) + \zeta(2,2)$, and $\zeta(2,1,1) = \zeta(4)$.

Solution. Define

$$\zeta(s_1, s_2, \cdots, s_k; x) \quad \sum_{n_1>n_2>\cdots>n_k>0} \frac{x_1^n}{n_1^{s_1} n_2^{s_2} \cdots n_r^{s_r}}, \tag{8.28}$$

for $s_1, s_2, \ldots, s_k$ nonnegative integers. We see that we are asked to compute $\zeta(3,1,3,1;1)$. Such a sum can be evaluated directly using the EZFace+ interface [83], which employs the Hölder convolution, giving us the numerical value

$$\begin{aligned}&0.0052295695635309601009306522838992315898904207846346355225\\&474489721488695446601500749754543248561040162 7\ldots.\end{aligned} \tag{8.29}$$

Alternatively, we may proceed using differential equations. It is fairly easy to see [51, Section 3.7] that

$$\begin{aligned}
\frac{d}{dx}\zeta(n_1, n_2, \cdots, n_r; x) \quad &= \quad \frac{1}{x}\zeta(n_1 - 1, n_2, \cdots, n_r; x), \qquad (n_1 > 1),\\
\frac{d}{dx}\zeta(n_1, n_2, \cdots, n_r; x) \quad &= \quad \frac{1}{1-x}\zeta(n_2, \cdots, n_r; x), \qquad (n_1 = 1),
\end{aligned}$$

with initial conditions $\zeta(n_1;0) = \zeta(n_1, n_2; 0) = \cdots \zeta(n_1, \cdots, n_r; 0) = 0$ and $\zeta(\cdot; x) \equiv 1$.

Solving

```
dsys1 > diff(y3131(x),x) = y2131(x)/x,
diff(y2131(x),x) = y1131(x)/x,
diff(y1131(x),x) = 1/(1-x)*y131(x),
diff(y131(x),x) = 1/(1-x)*y31(x),
diff(y31(x),x) = y21(x)/x,
diff(y21(x),x) = y11(x)/x,
diff(y11(x),x) = y1(x)/(1-x),
diff(y1(x),x) = 1/(1-x);
init1 = y3131(0) = 0,y2131(0) = 0, y1131(0) = 0,
   y131(0)=0,y31(0)=0,y21(0)=0,y11(0)=0,y1(0)=0;
```

in *Maple*, we obtain 0.005229569563518039612830536519667669502942 (this is valid to thirteen decimal places). *Maple*'s `identify` command is unable to identify portions of *this* number, and the Inverse Symbolic Calculator [84] does not return a result. It should be mentioned that both *Maple* and the ISC identified the constant $\zeta(3,1)$ (see the remark under the "history and context" heading). From the hint for this question, we know this is a single-term expression. Suspecting a form similar to $\zeta(3,1)$, we search for a constants c and d such that $\zeta(3,1,3,1) = c\pi^d$. This leads to $c = 1/81440 = 2/10!$ and $d = 8$.

Further history and context. We start with the simpler value, $\zeta(3,1)$. Notice that

$$-\log(1-x) = x + \frac{1}{2}x^2 + \frac{1}{3}x^3 + \cdots,$$

so

$$\begin{aligned} f(x) &= -\log(1-x)/(1-x) \;=\; x + (1+\frac{1}{2})x^2 + (1+\frac{1}{2}+\frac{1}{3})x^3 + \cdots \\ &= \sum_{n\geq k>0} \frac{x^n}{k}. \end{aligned}$$

As is used often in connection with such sums,

$$\frac{(-1)^{m+1}}{\Gamma(m)} \int_0^1 x^n \log^{m-1} x \, dx = \frac{1}{(n+1)^m},$$

so integrating f using this transform for $m = 3$, we obtain

$$\begin{aligned} \zeta(3,1) &= \frac{(-1)^4}{2} \int_0^1 f(x) \log^2 x \, dx \\ &= 0.2705808084277845478790009\,24\ldots. \end{aligned}$$

The corresponding generating function is

$$\sum_{n\ge 0} \zeta\left(\{3,1\}_n\right) x^{4n} \quad = \quad \frac{\cosh(\pi x) - \cos(\pi x)}{\pi^2 x^2},$$

equivalent to Zagier's conjectured identity

$$\zeta(\{3,1\}_n) = \frac{2\,\pi^{4n}}{(4n+2)}.$$

Here $\{3,1\}_n$ denotes n-fold concatenation of $\{3,1\}$.

The proof of this identity (see [51, p. 160]) derives from a remarkable factorization of the generating function in terms of hypergeometric functions:

$$\begin{aligned}\sum_{n\ge 0} \zeta(\{3,1\}_n) x^{4n} \quad &= \quad {}_2\mathrm{F}_1\left(x\frac{(1+i)}{2}, -x\frac{(1+i)}{2}; 1; 1\right) \\ &\quad \times {}_2\mathrm{F}_1\left(x\frac{(1-i)}{2}, -x\frac{(1-i)}{2}; 1; 1\right).\end{aligned}$$

Finally, it can be shown in various ways that

$$\zeta(\{3\}_n) \quad = \quad \zeta(\{2,1\}_n)$$

for all n, while a proof of the numerically-confirmed conjecture

$$\zeta(\{2,1\}_n) \quad \stackrel{?}{=} \quad 2^{3n}\,\zeta(\{-2,1\}_n) \tag{8.30}$$

remains elusive. The -2 indicates that the corresponding term alternates. Only the first case of (8.30), namely,

$$\sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} \quad = \quad 8 \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} \qquad (= \zeta(3)),$$

has a self-contained proof [51]. Indeed, the only other established case is

$$\sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} \sum_{p=1}^{m-1} \frac{1}{p^2} \sum_{q=1}^{p-1} \frac{1}{q} = 64 \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} \sum_{p=1}^{m-1} \frac{(-1)^p}{p^2} \sum_{q=1}^{p-1} \frac{1}{q}$$

$(= \zeta(3,3))$. This is an outcome of a complete set of equations for multivariate zeta values of depth four.

As we discussed in Chapter 1, there has been abundant evidence amassed to support identity (8.30) since it was found in 1996. This is the *only* identification of its type of an Euler sum with a distinct multivariate zeta function.

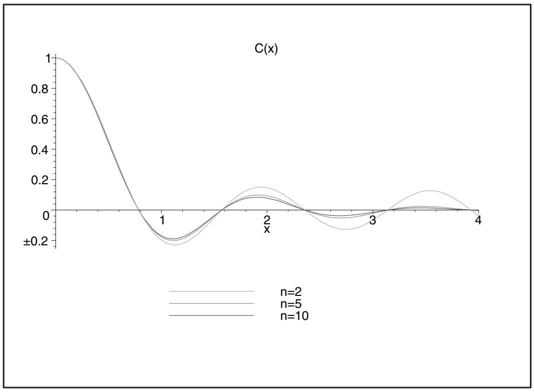


Figure 8.12. Approximations to $\prod_{n\geq 1}\cos(x/n)$.

8.7.2 $\pi/8$ or Not?

Problem 8. *Calculate*

$$\pi_2 = \int_0^\infty \cos(2x)\prod_{n=1}^\infty \cos\left(\frac{x}{n}\right)\,dx.$$

History and context. The challenge of showing that $\pi_2 < \pi/8$ was posed by Bernard Mares, Jr., along with the problem of demonstrating that

$$\pi_1 = \int_0^\infty \prod_{n=1}^\infty \cos\left(\frac{x}{n}\right)\,dx < \frac{\pi}{4}.$$

This is indeed true, although the error is remarkably small, as we shall see.

Solution. The computation of a high-precision numerical value for this integral is rather challenging, owing in part to the oscillatory behavior of $\prod_{n\geq 1}\cos(x/n)$, see Figure 8.12, but mostly because of the difficulty of computing high-precision evaluations of the integrand. Note that evaluating thousands of terms of the infinite product would produce only a few correct digits. Thus, it is necessary to rewrite the integrand in a form more suitable for computation as discussed in Chapter 3.

Let $f(x)$ signify the integrand. We can express $f(x)$ as

$$f(x) \quad = \quad \cos(2x)\left[\prod_1^m \cos(x/k)\right]\exp(f_m(x)), \tag{8.31}$$

where we choose m greater than x and where

$$f_m(x) = \sum_{k=m+1}^{\infty} \log\cos\left(\frac{x}{k}\right). \tag{8.32}$$

The kth summand can be expanded in a Taylor series [1, p. 75], as follows:

$$\log\cos\left(\frac{x}{k}\right) = \sum_{j=1}^{\infty} \frac{(-1)^j 2^{2j-1}(2^{2j}-1)B_{2j}}{j(2j)!}\left(\frac{x}{k}\right)^{2j},$$

in which B_{2j} are again Bernoulli numbers. Observe that since $k > m > x$ in (8.32), this series converges. We can then write

$$f_m(x) = \sum_{k=m+1}^{\infty} \sum_{j=1}^{\infty} \frac{(-1)^j 2^{2j-1}(2^{2j}-1)B_{2j}}{j(2j)!}\left(\frac{x}{k}\right)^{2j}. \tag{8.33}$$

After applying the classical identity (3.17), namely

$$B_{2j} = \frac{(-1)^{j+1}2(2j)!\zeta(2j)}{(2\pi)^{2j}},$$

and interchanging the sums, we obtain

$$f_m(x) = -\sum_{j=1}^{\infty} \frac{(2^{2j}-1)\zeta(2j)}{j\pi^{2j}}\left[\sum_{k=m+1}^{\infty} \frac{1}{k^{2j}}\right] x^{2j}.$$

Note that the inner sum can also be written in terms of the zeta function, as follows:

$$f_m(x) = -\sum_{j=1}^{\infty} \frac{(2^{2j}-1)\zeta(2j)}{j\pi^{2j}}\left[\zeta(2j) - \sum_{k=1}^{m} \frac{1}{k^{2j}}\right] x^{2j}.$$

This can now be reduced to a compact form for purposes of computation as

$$f_m(x) = -\sum_{j=1}^{\infty} a_j b_{j,m} x^{2j}, \tag{8.34}$$

where

$$a_j = \frac{(2^{2j}-1)\zeta(2j)}{j\pi^{2j}}, \tag{8.35}$$

$$b_{j,m} = \zeta(2j) - \sum_{k=1}^{m} 1/k^{2j}. \tag{8.36}$$

We remark that $\zeta(2j)$, a_j, and $b_{j,m}$ can all be precomputed, say for j up to some specified limit and for a variety of m. In our program, which computes this integral to 120-digit accuracy, we precompute $b_{j,m}$ for $m = 1, 2, 4, 8, 16, ..., 256$ and for j up to 300. During the quadrature computation, the function evaluation program picks m to be the first power of two greater than the argument x and then applies formulas (8.31) and (8.34). It is not necessary to compute $f(x)$ for x larger than 200, since for these large arguments $|f(x)| < 10^{-120}$ and thus may be presumed to be zero.

The computation of values of the Riemann zeta function can be done in various ways, but since what we really require is the entire set of values $\{\zeta(2j) : 1 \le j \le n\}$ for some n, we can use a convolution scheme described in [17]. It is important to note that the computation of both the zeta values and the $b_{j,m}$ must be done with a much higher working precision (in our program, we use 1600-digit precision) than the 120-digit precision required for the quadrature results, since the two terms being subtracted in formula (8.36) are very nearly equal. These values need to be calculated to a *relative* precision of 120 digits.

With this evaluation scheme for $f(x)$ in hand, the integrand in (8.31) can be integrated using, for instance, the tanh-sinh quadrature algorithm (see Section 3.4.1).

In spite of the substantial computation required to construct the zeta- and b-arrays, as well as the abscissas x_j and weights w_j needed for tanh-sinh quadrature, the entire calculation requires only about one minute on a 2004-era computer, using the ARPREC arbitrary precision software package [11]. The first hundred digits of the result are the following:

$$0.39269908169872415480783042290993786052464543418723159592681$$
$$22851620932471399385461790165127474553667777....$$

A *Mathematica* program capable of producing 100 digits of this constant is available on Michael Trott's website [267].

Using the Inverse Symbolic Calculator, for instance, one finds that this constant is likely to be $\pi/8$. But a careful comparison with a high-precision value of $\pi/8$, namely,

$$0.39269908169872415480783042290993786052464617492188822762186$$
$$80740384770507857761248285043531677646334 97...,$$

reveals that they are *not* equal—the two values differ by approximately 7.407×10^{-43}. Indeed, these two values are provably distinct. This follows from the fact that

$$\sum_{n=1}^{55} 1/(2n+1) \quad > \quad 2 > \sum_{n=1}^{54} 1/(2n+1).$$

See [51, Chapter 2] for additional details. We do not know a concise closed-form expression for this constant.

Further history and context. Recall the *sinc* function

$$\operatorname{sinc} x \quad = \quad \frac{\sin x}{x},$$

and consider the seven highly oscillatory integrals:

$$\begin{aligned}
I_1 &= \int_0^\infty \operatorname{sinc} x \, dx = \frac{\pi}{2}, \\
I_2 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc}\left(\frac{x}{3}\right) dx = \frac{\pi}{2}, \\
I_3 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc}\left(\frac{x}{3}\right) \operatorname{sinc}\left(\frac{x}{5}\right) dx = \frac{\pi}{2}, \\
&\vdots \\
I_6 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{11}\right) dx = \frac{\pi}{2}, \\
I_7 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{13}\right) dx = \frac{\pi}{2}.
\end{aligned}$$

It comes as something of a surprise, therefore, that

$$\begin{aligned}
I_8 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{15}\right) dx \\
&= \frac{467807924713440738696537864469}{935615849440640907310521750000}\pi \approx 0.499999999992646\pi.
\end{aligned}$$

When this was first discovered by a researcher, using a well-known computer algebra package, both he and the software vendor concluded there was a "bug" in the software. Not so! It is fairly easy to see that the limit of the sequence of such integrals is $2\pi_1$. Our analysis, via Parseval's theorem, links the integral

$$I_N \quad = \quad \int_0^\infty \operatorname{sinc}(a_1 x) \operatorname{sinc}(a_2 x) \cdots \operatorname{sinc}(a_N x) \, dx$$

with the volume of the polyhedron P_N described by

$$P_N \quad = \quad \{x : |\sum_{k=2}^{N} a_k x_k| \le a_1, |x_k| \le 1, 2 \le k \le N\},$$

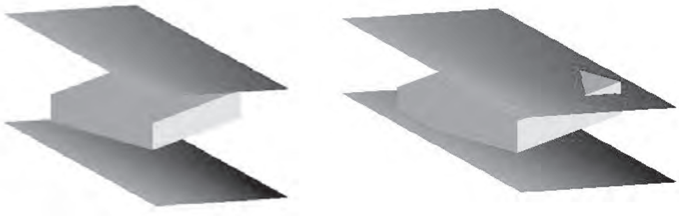


Figure 8.13. The "bite" in three dimensions.

for $x = (x_2, x_3, \cdots, x_N)$. If we let

$$C_N = \{(x_2, x_3, \cdots, x_N) : -1 \le x_k \le 1, 2 \le k \le N\},$$

then

$$I_N = \frac{\pi}{2a_1} \frac{\mathrm{Vol}(P_N)}{\mathrm{Vol}(C_N)}.$$

Thus, the value drops precisely when the constraint $\sum_{k=2}^{N} a_k x_k \le a_1$ becomes *active* and bites the hypercube C_N, as in Figure 8.13. That occurs when $\sum_{k=2}^{N} a_k > a_1$. In the foregoing,

$$\frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{13} < 1,$$

but on addition of the term $1/15$, the sum exceeds 1, the volume drops, and $I_N = \pi/2$ no longer holds. A similar analysis applies to π_2. Moreover, it is fortunate that we began with π_1 or the falsehood of $\pi_2 = 1/8$ would have been much harder to see.

Additional information on this problem is available at [278] http://mathworld.wolfram.com/InfiniteCosineProductIntegral.html and at http://mathworld.wolfram.com/BorweinIntegrals.html.

An interesting combinatorial analysis of such volumes and a useful historical discussion can be found in [209].

8.8 Last Words

As this book has tried to show, the horizons of experimental mathematics are in a period of rapid and exciting expansion. The changing environment both enlivens old mathematics (such as Hilbert's inequality) and allows insight on much newer topics (such as chaos games).

Year by year, what is possible for hybrid symbolic-numeric calculation changes. Consider, for $n = 1, 2, 3, \ldots$, the following *Ising susceptibility integrals* [18]:

$$\begin{aligned}
C_n &:= \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2}\frac{du_1}{u_1}\cdots\frac{du_n}{u_n}, \\
D_n &:= \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{\prod_{i<j}\left(\frac{u_i-u_j}{u_i+u_j}\right)^2}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2}\frac{du_1}{u_1}\cdots\frac{du_n}{u_n}, \\
E_n &:= \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \prod_{i<j}\left(\frac{u_i-u_j}{u_i+u_j}\right)^2 \frac{du_1}{u_1}\cdots\frac{du_n}{u_n}.
\end{aligned} \tag{8.37}$$

We discussed the C_n integrals briefly in Section 3.4. The first few values of the C_n integrals are known to be $C_1 = 2$, $C_2 = 1$, $C_3 = \mathrm{L}_{-3}(2)$, and $C_4 = 7\zeta(3)/12$. The first few values of the D_n integrals are $D_1 = 2$, $D_2 = 1/3$, $D_3 = 8 + 4\pi^2/3 - 27\,\mathrm{L}_{-3}(2)$, and $D_4 = 4\pi^2/9 - 1/6 - 7\zeta(3)/2$. The D_4 value is due to McCoy, Tracy, and Wu in the late seventies, while no higher symbolic value has yet been resolved.

The first few values of the E_n constants are known to be $E_1 = 2$, $E_2 = 6 - 8\log 2$, and $E_3 = 10 - 2\pi^2 - 8\log 2 + 32\log^2 2$. The next two are

$$\begin{aligned}
E_4 &= 22 - 82\zeta(3) - 24\log 2 + 176\log^2 2 - 256(\log^3 2)/3 \\
&\quad + 16\pi^2\log 2 - 22\pi^2/3, \\
E_5 &\stackrel{?}{=} 42 - 1984\,\mathrm{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3)\log 2 \\
&\quad + 40\pi^2\log^2 2 - 62\pi^2/3 + 40(\pi^2\log 2)/3 + 88\log^4 2 \\
&\quad + 464\log^2 2 - 40\log 2.
\end{aligned} \tag{8.38}$$

All of this is detailed in [18].

The result (8.38) is a recent experimental discovery, based on the computation of a 240-digit numerical value of E_5, which required two hours on 64 CPUs of a highly parallel computer system at Virginia Tech, followed by a PSLQ program that produced the experimental evaluation above. The question mark is used because no proof is known as of this date. Figure 2.1 in Section 2.3 is a plot of the progress of this PSLQ run—note that at the final iteration (iteration 199) the size of the smallest entry of the reduced x vector precipitously drops 180 orders of magnitude to 10^{-240}, which is the "epsilon" in the 240-digit arithmetic being used in this calculation. Such a large drop suggests that it is exceedingly unlikely that (8.38) is an artifact of numerical error.

Correspondingly, an eighteen-hour computation on 256 processors on an IBM parallel computer system at the Lawrence Berkeley Laboratory returned the following numerical value of D_5:

```
0.002484605762340315479950509153909749635060677642487516158707692161
```

This far-from-elementary 500-digit calculation (as well as the calculation of E_5 and some other constants) is described in [18], as are some extensive but unsuccessful integer relation hunts. In consequence, we end with a challenge to the reader to obtain a closed form for D_5 from this now substantial numeric data. As the Frenchman d'Alembert remarked *"L'algèbre est genereuse, elle donne souvent plus qu'on lui demande."*[4] With any luck he was right in this case.

[4]Edward Kasner wrote in [175] "The formulas move in advance of thought, while the intuition often lags behind; in the oft-quoted words of d'Alembert, '*L'algèbre est genereuse, elle donne souvent plus qu'on lui demande.*'"

9 Exercises

> Keynes distrusted intellectual rigour of the Ricardian type as likely to get in the way of original thinking and saw that it was not uncommon to hit on a valid conclusion before finding a logical path to it.
>
> —Sir Alec Cairncross[1]

This chapter contains nine sections. The first eight sections contain exercises generally relating to the corresponding chapter, while the ninth contains a large compendium of extras. A significant number of the exercises originated in the pages of the *American Mathematical Monthly* (AMM) or from the annual Putnam competition. They provide an interesting opportunity to see how the art of problem solving changes in the presence of modern computers and good mathematical software. In each case, a few lines of computer algebra code either provides the solution, suggests an approach, or at least confirms the answer.

Exercises for Chapter 1

1. (AMM Problem 11197.) Prove that, for all positive real numbers with $x^2+y^2+z^2=1$, one has

$$\frac{x}{1-x^{2n}}+\frac{y}{1-y^{2n}}+\frac{z}{1-z^{2n}} \geq \frac{(2n+1)^{1+1/(2n)}}{2n},$$

   for all positive integer n.

   Hint: $1/(t(1-t^{2n})) \geq (2n+1)^{1+1/(2n)}/(2n)$ for $0<t<1$.

2. Nick Trefethen's fourth digit-challenge problem was given as (1.5) in Chapter 1. Find a numerical or graphical method to obtain ten good digits of the solution that occurs near $(-0.15, 0.29, -.028)$ with value -3.32834.

3. (A problem for Ramanujan [137, p. 201].) Find all integers n such that for some $1 \leq m \leq n$ one has

$$1+2+\cdots+(m-1)=(m+1)+(m+2)+\cdots+n.$$

   Hint: Compare Sloane's sequence A001109.

[1] In "Keynes the Man," written on the 50th anniversary of Keynes' death. *The Economist*, April 20, 1996.

4. Prove that

$$0 < \frac{1}{3164}\int_0^1 \frac{x^8(1-x)^8\left(25+816x^2\right)}{1+x^2}\,dx = \frac{355}{113} - \pi,$$

and derive the estimate that

$$\frac{355}{113} - \frac{911}{2630555928} < \pi < \frac{355}{113} - \frac{911}{5261111856}.$$

5. (Powers of arcsin.) The formula for $\arcsin^2(x)$ discovered in the text is the first example of a family of formulas that can be experimentally discovered as is described in [63].

   (a) Show that

$$\arcsin^4\left(\frac{x}{2}\right) = \frac{3}{2}\sum_{k=1}^{\infty}\left\{\sum_{m=1}^{k-1}\frac{1}{m^2}\right\}\frac{x^{2k}}{\binom{2k}{k}k^2}.$$

   More generally, show that for $|x| \le 2$ and $N = 1, 2, \ldots$

$$\frac{\arcsin^{2N}\left(\frac{x}{2}\right)}{(2N)!} = \sum_{k=1}^{\infty}\frac{H_N(k)}{\binom{2k}{k}k^2}x^{2k}, \tag{9.1}$$

   where $H_1(k) = 1/4$ and

$$H_{N+1}(k) := \sum_{n_1=1}^{k-1}\frac{1}{(2n_1)^2}\sum_{n_2=1}^{n_1-1}\frac{1}{(2n_2)^2}\cdots\sum_{n_N=1}^{n_{N-1}-1}\frac{1}{(2n_N)^2}.$$

   (b) Show that for $|x| \le 2$ and $N = 0, 1, 2, \ldots$

$$\frac{\arcsin^{2N+1}\left(\frac{x}{2}\right)}{(2N+1)!} = \sum_{k=0}^{\infty}\frac{G_N(k)\binom{2k}{k}}{2(2k+1)4^{2k}}x^{2k+1}, \tag{9.2}$$

   where $G_0(k) = 1$ and

$$G_N(k) := \sum_{n_1=0}^{k-1}\frac{1}{(2n_1+1)^2}\sum_{n_2=0}^{n_1-1}\frac{1}{(2n_2+1)^2}\cdots\sum_{n_N=0}^{n_{N-1}-1}\frac{1}{(2n_N+1)^2}.$$

Proof: The formulas for $\arcsin^k(x)$ with $1 \le k \le 4$ are given on pages 262–263 of [33]. Berndt's proof implicitly gives the desired result since it establishes that for all a

$$e^{a\arcsin(x)} = \sum_{n=0}^{\infty} c_n \frac{x^n}{n!}, \tag{9.3}$$

where

$$c_{2n+1} = a\prod_{k=1}^{n}\left(a^2+(2k-1)^2\right), \qquad c_{2n} = \prod_{k=1}^{n}\left(a^2+(2k-2)^2\right).$$

Now expanding the power of a^n on each side of (9.3) provides the asserted formula. Another proof can be obtained from the hypergeometric identity

$$\frac{\sin(ax)}{a\sin(x)} = {}_2F_1\left(\frac{1+a}{2}, \frac{1-a}{2}; \frac{3}{2}; \sin^2(x)\right)$$

given in [52, Exercise 16, p. 189]. □

Maple can prove identities such as (9.3), as the following code shows.

```
ce:=n->product(a^2+(2*k)^2,k=0..n-1):
co:=n->a*product(a^2+(2*k+1)^2,k=0..n-1):
sum(ce(n)*x^(2*n)/(2*n)!,n=0..infinity) assuming x>0;
simplify(expand(sum(co(n)*x^(2*n+1)/(2*n+1)!,n=0..infinity)))
  assuming x>0;
```

This outputs $\cosh(a\arcsin(x))$ and $\sinh(a\arcsin(x))$.

6. (A proof of Knuth's problem.) 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 the slowly convergent infinite sum

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

discussed in Chapter 1. Evidently, the *Maple* software knew something that we did not. Looking under the hood, we found *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 experimental identity, together with an obvious allusion to Stirling's formula in the original problem. This led us to conjecture the identity

$$\sum_{k=1}^{\infty}\left(\frac{1}{\sqrt{2\pi k}} - \frac{(1/2)_{k-1}}{(k-1)!\sqrt{2}}\right) = \frac{1}{\sqrt{2\pi}}\zeta\left(\frac{1}{2}\right), \tag{9.4}$$

where $(x)_n$ denotes the rising factorial or Pochhammer function $x(x+1)\cdots(x+n-1)$, and where the binomial coefficients in (9.4) 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

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

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. □

Such *instrumental* use of the computer is one of the most exciting features of experimental mathematics. The next three exercises explore the partition function and follow material in [52]; see also [51].

7. Euler's pentagonal number theorem is

$$Q(q) := \prod_{n\geq 1}(1-q^n) = \sum_{n=-\infty}^{\infty}(-1)^n q^{(3n+1)n/2}. \tag{9.5}$$

One would be less prone to look at Q on the way to the partition function today when computation is very snappy. Determine empirically the series for $Q^3(q)$.

8. Jacobi's triple product in general form is

$$\prod_{n\geq 1}(1+xq^{2n-1})(1+x^{-1}q^{2n-1})(1-q^{2n}) = \sum_{n=-\infty}^{\infty} x^n q^{n^2}. \tag{9.6}$$

Deduce from (9.6) the pentagonal number theorem of the previous exercise and that

$$\left(\sum_{n=-\infty}^{\infty}(-1)^n q^{(3n+1)n/2}\right)^3 = \sum_{m=0}^{\infty}(2m+1)(-1)^m q^{m(m+1)/2}. \tag{9.7}$$

9. (Modular properties of the partition function.)

   (a) Prove that the partition function of $5n+4$ is divisible by 5.

   Proof sketch: With Q as in (9.5), we obtain

$$\begin{aligned} qQ^4(q) &= q\,Q(q)Q^3(q) \qquad (9.8)\\ &= \sum_{m\geq 0}\sum_{n=-\infty}^{\infty}(-1)^{n+m}(2m+1)q^{1+(3n+1)n/2+m(m+1)/2} \end{aligned}$$

   from the triple product and pentagonal number theorems in Problems 7 and 8. Now consider when k is a multiple of 5, and discover that this can only happen if $2m+1$ is divisible by 5 as is the coefficient of q^{5m+5} in $qQ^4(q)$. Then, by the binomial theorem,

$$(1-q)^{-5} \equiv (1-q^5)^{-1} \quad \text{mod} 5.$$

Consequently, the coefficient of the corresponding term in $qQ(q^5)/Q(q)$ is divisible by 5. Finally,

$$q + \sum_{n>1} p(n-1)q^n = qQ^{-1}(q) = \frac{qQ(q^5)}{Q(q)} \prod_{m=1}^{\infty} \sum_{n=0}^{\infty} q^{5mn},$$

as claimed. □

(b) Try to extend this argument to show $p(7n+6)$ is divisible by 7.

The next three exercises are taken from [57] where many other such results may be found. We wish to show

$$\zeta(2,1) := \sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} = \sum_{n=1}^{\infty} \frac{1}{n^3} = \zeta(3) \quad \text{and} \tag{9.9}$$

$$\zeta(2,1) = 8 \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} =: 8\,\zeta(-2,1). \tag{9.10}$$

10. (Two proofs that $\zeta(2,1) = \zeta(3)$.)

(a) A really quick proof of (9.9) considers

$$S := \sum_{n,k>0} \frac{1}{nk(n+k)} = \sum_{n,k>0} \frac{1}{n^2}\left(\frac{1}{k} - \frac{1}{n+k}\right) = \sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{k=1}^{n} \frac{1}{k}$$
$$= \zeta(3) + \zeta(2,1). \tag{9.11}$$

On the other hand, by symmetry,

$$S = \sum_{n,k>0} \left(\frac{1}{n} + \frac{1}{k}\right) \frac{1}{(n+k)^2} = \sum_{n,k>0} \frac{1}{n(n+k)^2} + \sum_{n,k>0} \frac{1}{k(n+k)^2}$$
$$= 2\zeta(2,1).$$

(b) Show that

$$\zeta(3) = \int_0^1 (\log x) \log(1-x) \frac{dx}{x}. \tag{9.12}$$

Hint: Let $\varepsilon > 0$. Expand the integrand to get

$$\sum_{n=1}^{\infty} \frac{1}{(n+\varepsilon)^2} = \int_0^1 \int_0^1 \frac{(xy)^{\varepsilon}}{1-xy}\, dx\, dy.$$

Differentiate with respect to ε, and let $\varepsilon = 0$ to obtain

$$\zeta(3) = -\frac{1}{2} \int_0^1 \int_0^1 \frac{\log(xy)}{1-xy}\, dx\, dy$$
$$= -\frac{1}{2} \int_0^1 \int_0^1 \frac{\log x + \log y}{1-xy}\, dx\, dy$$
$$= -\int_0^1 \int_0^1 \frac{\log x}{1-xy}\, dx$$

by symmetry. Now integrate with respect to y to get (9.12).

(c) Hence,

$$\begin{aligned}2\zeta(3) &= \int_0^1 \frac{\log^2 x}{1-x}\,dx \\ &= \int_0^1 \log^2(1-x)\,\frac{dx}{x} = \sum_{n,k>0} \int_0^1 \frac{x^{n+k-1}}{nk}\,dx \\ &= \sum_{n,k>0} \frac{1}{nk(n+k)} = \zeta(2,1)+\zeta(3)\end{aligned}$$

on appealing to the first half of the first proof.

11. (A proof that $8\,\zeta(-2,1) = \zeta(2,1)$.) Let

$$J(x) := \sum_{n>k>0} \frac{x^n}{n^2 k}, \qquad 0 \le x \le 1.$$

(a) Show that

$$J(-x) = -J(x) + \frac{1}{4}J(x^2) + J\left(\frac{2x}{x+1}\right) - \frac{1}{8}J\left(\frac{4x}{(x+1)^2}\right). \tag{9.13}$$

Hint: Differentiate.

(b) Putting $x=1$ gives $8\,J(-1) = J(1)$ immediately, which is (9.10).

Further proofs may be found in the Exercises for Chapter 8.

12. (AMM Problem 11103, October 2004.) Show that for positive integer n

$$2^{1-n} \sum_{k=1}^{n} \frac{\binom{n}{2k-1}}{2k-1} = \sum_{k=1}^{n} \frac{1}{k\binom{n}{k}}.$$

Solution. We show that the ordinary generating function of each side is the same. Indeed, applying the binomial theorem while interchanging sum and integral allows one to write

$$\begin{aligned}2\sum_{n=1}^{\infty}\sum_{k=1}^{n} \frac{\binom{n}{2k-1}}{2k-1}\left(\frac{y}{2}\right)^n &= \int_0^1 \frac{\sum_{n=1}^{\infty}\left(\frac{y(1+t)}{2}\right)^n - \left(\frac{y(1-t)}{2}\right)^n}{t}\,dt \\ &= \int_0^1 \frac{4y}{(y+yt-2)(y-yt-2)}\,dt \\ &= \frac{-\log(1-y)}{1-y/2}.\end{aligned} \tag{9.14}$$

Also, using the Beta function to write $1/(k\binom{n}{k})$ as $\int_0^1 t^{k-1}(1-t)^{n-k}\,dt$ produces

$$\begin{aligned}\sum_{n=1}^{\infty}\sum_{k=1}^{n} \frac{1}{k\binom{n}{k}}\,y^n &= \int_0^1 \frac{\sum_{n=1}^{\infty}\{t^n-(1-t)^n\}}{2t-1}\,y^n\,dt \\ &= \int_0^1 \frac{y}{(1+yt-y)(1-yt)}\,dt \\ &= \frac{-\log(1-y)}{1-y/2}.\end{aligned} \tag{9.15}$$

Exercises for Chapter 2

1. (Arctan formula for π.) Find rational coefficients a_i such that the identity

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

holds. Also show that an identity with even simpler coefficients exists if $\arctan 1/239$ is included as one of the terms on the RHS.

2. (BBP formula for $\zeta(3)$.) The constant $\zeta(3)$ can be written as the BBP series

$$\zeta(3) = \frac{1}{a_0}\sum_{k=0}^{\infty}\frac{1}{2^{12k}}\sum_{j=1}^{23}\frac{a_j}{(24k+j)^3}$$

for certain integers a_i. Find the integers a_i, in lowest terms.

3. (BBP formula for arctan(4/5).) The constant $\arctan(4/5)$ can be written as the BBP series

$$\arctan\left(\frac{4}{5}\right) = \frac{1}{a_0}\sum_{k=0}^{\infty}\frac{1}{2^{20k}}\sum_{j=1}^{39}\frac{a_j}{40k+j}$$

for certain integers a_i. Find the integers a_i, in lowest terms.

4. (Digit frequencies.) Calculate π, $\sqrt{2}$, e, log2, and log10 to 100,000 digits, and then tabulate the ten single-digit frequencies and the 100 double-digit frequencies. One statistical procedure for testing the hypothesis that the empirical frequencies of n-long strings of digits are random is the χ^2 test. The χ^2 statistic of the k observations $X_1, X_2, \cdots, X_k$ is defined as

$$\chi^2 = \sum_{i=1}^{k}\frac{(X_i - E_i)^2}{E_i},$$

where E_i is the expected value of the random variable X_i. In this case, $k = 10$ for single-digit frequencies (100 for double-digit frequencies), $E_i = 10^{-n}d$ for all i (here $d = 100{,}000$), and (X_i) are the observed digit counts (or double-digit counts). The mean of the χ^2 statistic is $k-1$, and its standard deviation is $\sqrt{2(k-1)}$.

5. (BBP sequence for π.) A constant α is said to be b-normal if and only if for every $m > 1$, every string of length m appears, in the base-b expansion of α, with limiting frequency b^{-m}. It is shown in [24] that the hexadecimal-normality of π reduces to the question of whether the iteration $x_0 = 0$,

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

is a uniform pseudorandom number generator in the interval $(0, 1)$.

Using high-precision arithmetic software, calculate successive iterates of this sequence, up to say 1000 terms, and then tabulate the frequency of appearance of these iterates in the sixteen subintervals $[0, 1/16), [1/16, 2/16), \cdots, [15/16, 1]$, labeled 0, 1, 2, ..., 9, A, B, C, D, E, F as in hexadecimal digit notation. Then, use the chi-square test mentioned in the previous exercise to test the hypothesis that the iterates of the BBP sequence are uniformly distributed in the unit interval.

Also, examine the sequence of hexadecimal digits produced by this process. Do you recognize it?

Hint: Numerically evaluate this sequence as a hexadecimal number, where the "decimal" point precedes the first digit generated. (Also, consult Example 1.10 again.)

6. Show that this infinite series converges:

$$\sum_{n=1}^{\infty} \frac{(2 + \sin n)^n}{n 3^n}.$$

Hint: Experiment numerically with the series to see if any insight can be gained—the answer is probably not. Then, as suggested by Ravi Boppana, apply the following irrationality result of Hata [164] that extends work of Mahler [52]: For every sufficiently large integer q and every integer p, we have

$$\left|\pi - \frac{p}{q}\right| \geq \frac{1}{q^9}.$$

This irrationality estimate for π means that $\sin n$ cannot be close to unity very often. This problem was posed as an open problem in [50].

7. (AMM Problem 11164, May 2005.) Evaluate

$$\sum_{k=1}^{n} (-1)^{k+1} \binom{n}{k} \sum_{i=1}^{k} \frac{\sum_{j=1}^{i} 1/j}{i}$$

for $n = 1, 2, \ldots$.

Hint: Sum the first few terms.

8. (Trigonometric integrals.) Evaluate $A_n B_n$ for $n = 1, 2, \ldots$ when

$$A_n := \int_{-\infty}^{\infty} \frac{\sin(\pi x)}{\pi x} \prod_{k=1}^{n} \left(1 - \frac{x^2}{k^2}\right)^{-1} dx,$$

$$B_n := \int_{-\infty}^{\infty} \frac{\cos(\pi x)}{\pi} \prod_{k=1}^{n} \left(1 - \frac{x^2}{(k-1/2)^2}\right)^{-1} dx.$$

Hint: Evaluate the first few terms.

9. (A golden example.) Evaluate the following sum:

$$\Phi := \sum_{k=0}^{\infty} \left\{ \frac{G^2}{(5k+1)^2} - \frac{G}{(5k+2)^2} - \frac{G^2}{(5k+3)^2} + \frac{G^5}{(5k+4)^2} + \frac{2\,G^5}{(5k+5)^2} \right\} g^{5k} \tag{9.16}$$

where $g := (\sqrt{5}-1)/2$ is the *golden ratio* and $G := (\sqrt{5}+1)/2 = g^{-1}$.
Hint: The answer, $\Phi = \pi^2/50$, was discovered empirically by Benoit Cloitre using integer relation methods. In the irrational base g, the constant Φ has digits independently computable since (9.16) gives an identity of BBP type. (See [50, Chapter 4].)

(a) With computer algebra assistance, work backwards to needing to show that

$$\Phi = \operatorname{Re}\operatorname{Li}_2\left(2\cos(\theta)\, e^{\pi i \theta}\right)$$

for $\theta := 2\pi/5$, where $\operatorname{Li}_2(x) = \sum_{n=1}^{\infty} x^n/n^2$ is the dilogarithm.

(b) Show that for all real θ

$$\sum_{n=1}^{\infty} \frac{\cos(n\theta)\,(2\cos(\theta))^n}{n^2} = \left(\frac{\pi}{2} - \theta\right)^2.$$

This is equation (5.17) in L. Lewin's book on dilogarithms [198] and is relatively easy to obtain.

(c) Show that $\theta = 2\pi/5$ makes $2\cos(\theta) = (\sqrt{5}-1)/2 = g$. Moreover $2\cos(n\theta)$ takes the values $2, g, -1/g, -1/g, g$ modulo 5. Thus, obtain (9.16).

(d) Any other rational multiple of π has a like form—nicest when $2\cos(n\theta)$ is rational or quadratic. Thus, with $\theta := \pi/3, 2\pi/3$, we obtain, inter alia, an evaluation of $\zeta(2)$. With $\theta := 3\pi/8, 5\pi/12$, we obtain nice convergent identities.

10. (AMM Problem 11103, October 2004: a second proof.) In Exercise 12 for Chapter 1 we explored this problem. Show that for positive integer n

$$2^{1-n} \sum_{k=1}^{n} \frac{\binom{n}{2k-1}}{2k-1} = \sum_{k=1}^{n} \frac{1}{k\binom{n}{k}}.$$

(a) Use integer relation methods to predict the recursion

$$(n+1)\,u_n - (2n+4)\,u_{n+1} + (3n+4)\,u_{n+2} = 0 \tag{9.17}$$

for the hypergeometric sum on the right-hand side of the requested identity.

(b) Use the Wilf-Zeilberger method to prove this.

(c) Prove that the left-hand series satisfies the same recursion (9.17) and initial conditions and hence coincides with the right,

11. (A difficult limit.) This originates with Mike Hirschhorn's treatment in [167] of a solution to AMM problem 10886.

Prove that

$$\gamma_n \quad := \quad \frac{1}{2^n \binom{2n}{n}} \, \frac{\sum_{k=0}^{n} \frac{\binom{n}{k}}{n+k}}{\sum_{k=0}^{n} (-1)^k \, \frac{\binom{n}{k}}{n+k}}$$

converges as n goes to ∞, and determine the limit as follows:

(a) Compute enough terms to make plausible that the limit is $2/3$—with error roughly $2/(27n)$.

(b) Verify that also

$$\gamma_n = n\,2^{-n} \int_0^1 t^{n-1}(1+t)^n \, dt.$$

(c) Show that

$$\sum_{n=0}^{\infty} \gamma_n x^n \quad = \quad \int_0^1 \frac{2(1+t)x}{\left(2-(t+t^2)x\right)^2} \, dt \geq \frac{x(3-x)}{(1-x)(4-x)}.$$

(d) Hence, show that $\gamma_n \geq 2/3 + 4^{-n}/3$.

(e) Use Wilf-Zeilberger methods to verify a third representation:

$$\gamma_n = \frac{1}{\binom{2n}{n}} \sum_{k \geq 0} 2^{-k} \binom{2n-1-k}{n-1}.$$

(f) Finally, estimate that

$$\gamma_n \leq \frac{1}{2} + \frac{2n}{2n-1} \sum_{k \geq 1} 2^{-(2k+1)} \leq \frac{2}{3} + \frac{6}{2n-1}.$$

12. (Integer relations as integer knapsack problems.) An *integer knapsack problem* is an integer programming problem with one constraint, such as

$$\min \sum_{k=1}^{N} \omega_k \quad \text{subject to} \quad \sum_{k=1}^{N} \omega_k \alpha_k \quad = \quad \beta, \, \omega_1 \geq 0, \omega_2 \geq 0, \ldots, \omega_N \geq 0, \tag{9.18}$$

where the nonnegative weights ω_k are required to be integers. If we view β as a quantity that we wish to express in terms of real (or vector) quantities $\mathscr{A} := \{\alpha_1, \alpha_2 \ldots, \alpha_N\}$, then (9.18) will solve a positive integer relation problem. Since there are excellent integer programming algorithms, it makes sense to investigate this as a tool in various settings:

(a) *When all signs are known* as when one is checking a known formula but has forgotten the exact constants, e.g., in Machin's formula

$$\arctan(1) = \omega_1 \arctan\left(\frac{1}{5}\right) - \omega_2 \arctan\left(\frac{1}{239}\right)$$

or Euler's formula

$$\arctan(1) = \omega_1 \arctan\left(\frac{1}{2}\right) + \omega_2 \arctan\left(\frac{1}{5}\right) + \omega_3 \arctan\left(\frac{1}{8}\right).$$

(b) *When all signs are anticipated,* this can also be something provable. Indeed, for $\zeta(4N+1)$, very pretty three-term representations arise from a couple of PSLQ observations by Simon Plouffe.

For $N = 1, 2, 3 \ldots$

$$\left\{2 - (-4)^{-N}\right\} \sum_{k=1}^{\infty} \frac{\coth(k\pi)}{k^{4N+1}} - (-4)^{-2N} \sum_{k=1}^{\infty} \frac{\tanh(k\pi)}{k^{4N+1}} \\ = Q_N \times \pi^{4N+1},$$

where the quantity Q_N is the explicit rational

$$Q_N := \sum_{k=0}^{2N+1} \frac{B_{4N+2-2k} B_{2k}}{(4N+2-2k)!(2k)!} \left\{(-1)^{\binom{k}{2}} (-4)^N 2^k + (-4)^k\right\}.$$

On substituting

$$\tanh x = 1 - \frac{2}{\exp(2x)+1} \quad \text{and} \quad \coth x = 1 + \frac{2}{\exp(2x)-1},$$

one may solve for $\zeta(4N+1)$. We list two examples:

$$\zeta(5) = \frac{1}{294}\pi^5 - \frac{2}{35} \sum_{k=1}^{\infty} \frac{1}{(1+e^{2k\pi})k^5} + \frac{72}{35} \sum_{k=1}^{\infty} \frac{1}{(1-e^{2k\pi})k^5}$$

and

$$\zeta(9) = \frac{125}{3704778}\pi^9 - \frac{2}{495} \sum_{k=1}^{\infty} \frac{1}{(1+e^{2k\pi})k^9} + \frac{992}{495} \sum_{k=1}^{\infty} \frac{1}{(1-e^{2k\pi})k^9}.$$

This sign pattern sustains for all $\zeta(4N+1)$ and allows one to determine sufficient coefficients to validate or discover the general formula.

(c) The well-known series for $\arcsin^2 x$ generalizes fully, as we saw in the Exercises for Chapter 1. The seed identity is well known:

$$\arcsin^2\left(\frac{x}{2}\right) = \frac{1}{2}\sum_{k=1}^{\infty} \frac{x^{2k}}{\binom{2k}{k}k^2}. \tag{9.19}$$

The second, slightly rewritten identity is less well known:

$$\arcsin^4\left(\frac{x}{2}\right) = \frac{3}{2}\sum_{k=1}^{\infty}\left\{\sum_{m=1}^{k-1}\frac{1}{m^2}\right\}\frac{x^{2k}}{\binom{2k}{k}k^2},$$

and when compared, they suggest the third and fourth—subsequently confirmed numerically—by the prior, if flimsy, pattern:

$$\arcsin^6\left(\frac{x}{2}\right) = \frac{45}{4}\sum_{k=1}^{\infty}\left\{\sum_{m=1}^{k-1}\frac{1}{m^2}\sum_{n=1}^{m-1}\frac{1}{n^2}\right\}\frac{x^{2k}}{\binom{2k}{k}k^2},$$

$$\arcsin^8\left(\frac{x}{2}\right) = \frac{315}{2}\sum_{k=1}^{\infty}\left\{\sum_{m=1}^{k-1}\frac{1}{m^2}\sum_{n=1}^{m-1}\frac{1}{n^2}\sum_{p=1}^{n-1}\frac{1}{p^2}\right\}\frac{x^{2k}}{\binom{2k}{k}k^2}.$$

In this case all signs are positive and positive integer relation methods again apply. These relations were found by hunting over larger sets of multi-dimensional sums.

(d) In particular, for $N = 1, 2, \ldots$

$$\sum_{k=1}^{\infty}\frac{H_N(k)}{\binom{2k}{k}k^2} = \frac{\pi^{2N}}{6^{2N}(2N)!},$$

with the $H_N(k)$ multi-dimensional harmonic numbers. The first few right-hand side values are

$$\frac{1}{72}\pi^2, \quad \frac{1}{31104}\pi^4, \quad \frac{1}{33592320}\pi^6, \quad \text{and} \quad \frac{1}{67722117120}\pi^8.$$

(e) Let

$$\mathscr{L}(s,t) := \sum_{n>m>0}\frac{(-1)^{n-1}}{n^s}\frac{\chi_3(m)}{m^t},$$

where χ_3 is the character modulo 3 (which is ± 1 when $n \equiv \pm 1$ modulo 3 and is zero otherwise). Then,

$$\begin{aligned}\mathscr{L}(2N+1,1) = {} & \frac{L_{-3}(2N+2)}{4^{1+N}} - \frac{1+4^{-N}}{2}L_{-3}(2N+1)\log(3)\\ & + \sum_{k=1}^{N}\frac{1-3^{-2N+2k}}{2}L_{-3}(2N-2k+2)\,\alpha(2k)\\ & - \sum_{k=1}^{N}\frac{1-9^{-k}}{1-4^{-k}}\,\frac{1+4^{-N+k}}{2}\\ & \qquad \times L_{-3}(2N-2k+1)\,\alpha(2k+1)\\ & - 2L_{-3}(1)\,\alpha(2N+1),\end{aligned} \tag{9.20}$$

where α is the alternating zeta function and L_{-3} is the *primitive L-series modulo 3*. One first numerically evaluates such $\mathscr{Z}$ sums as integrals via

$$\mathscr{Z}(s,1) = \int_0^1 \frac{\mathrm{L}_{-3}(s:-x)}{1+x}\,dx,$$

where

$$L_3(s:x) = \sum_{m=1}^{\infty} \frac{\chi_3(m)x^m}{m^s} = xxx$$

and $\chi_3(n)$ repeats $1,-1,0$ modulo three. Notice also that the sign pattern will become obvious well before the exact form of the coefficients—especially those in the third line of (9.20). This sort of evaluation, and much more about character Euler sums, may be pursued in [71].

(f) *For small* $\mathscr{A}$, say $N<6$, one may try all 2^N sign permutations. For example, one may remember that

$$\Gamma(2x) = \pi^{\alpha(x)} 2^{\beta x+\gamma}\Gamma(x)\Gamma(x+1/2),$$

but not remember the rational constants. Taking logarithms and using PSLQ at a few rational values of x will recreate the formula. Likewise, *for medium sized* $\mathscr{A}$, where one knows or anticipates many of the signs, one may fix those signs and search over all remaining combinations.

Finally, one may well have *under-determined systems* (with too many relations) and wish to select a relation with a predetermined sign configuration.

13. (Apéry formulas.) This exercise is due to Margo Kondratieva.

(a) Show that (a formula originally found by Markov in 1890)

$$\sum_{n=0}^{\infty} \frac{1}{(n+a)^3} = \frac{1}{4}\sum_{n=0}^{\infty} \frac{(-1)^n\,(n!)^6}{(2n+1)!} \times \frac{\left(5\,(n+1)^2 + 6\,(a-1)\,(n+1) + 2\,(a-1)^2\right)}{\prod_{k=0}^{n}(a+k)^4}.$$

(b) Rederive Apéry's formula for $\zeta(3)$. Note: *Maple* establishes this identity as

$$-1/2\,\Psi(2,a) = -1/2\,\Psi(2,a) - \zeta(3) + 5/4\,{}_4\mathrm{F}_3\left([1,1,1,1],[3/2,2,2],-1/4\right).$$

(c) Prove the following identity:

$$\zeta(4) = -\sum_{m=1}^{\infty}\frac{(-1)^{m-1}}{\binom{2m}{m}m^4} + \frac{10}{3}\sum_{m=1}^{\infty}\frac{(-1)^{m-1}\sum_{k=1}^{m}\frac{1}{k}}{\binom{2m}{m}m^3}.$$

14. (Box integrals.) Evaluate

$$B_N := \int_0^1 \cdots \int_0^1 \left(\sum_{k=1}^{N} x_k^2\right)^{1/2} dx_1 \cdots dx_n,$$

Answer: $B_2 = \sqrt{2}/3 + \log(\sqrt{2}+1)/3$, and $B_3 = \sqrt{3}/4 + \log(2+\sqrt{3})/2 - \pi/24$. Can you recognize or evaluate B_4 or B_5?

15. (Singular value theory.) This exercise is due to Jonathan Borwein and John Zucker. We begin by paraphrasing some background that is elaborated in [52]. Let $K(k)$ be the *complete elliptic integral of the first kind* given by

$$K(k) \quad = \quad \int_0^1 \frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}},$$

where k denotes the modulus. For a given positive integer N consider the equation

$$\frac{K'(k)}{K(k)} \quad = \quad \sqrt{N}, \tag{9.21}$$

where $K'(k) \equiv K(k')$ and $k' \equiv (1-k^2)^{\frac{1}{2}}$ is the complimentary modulus. When $k \in (0,1)$, it is known that (9.21) has a unique solution $k \equiv k_N$ which is an *algebraic* number, often but not always solvable in radicals [52, Section 9.1].

As described in [52], Selberg and Chowla proved that $K(k_N) \equiv K[N]$ could be expressed in terms of products of Γ functions, algebraic numbers, and powers of π. Borwein and Zucker [72] subsequently showed that these formulas were much simplified if they were expressed in terms of the Euler Beta function $B(p,q)$; see (7.75). Further, for all $N = 1,2$ (mod 4), an extra simplification was achieved since they found that only the *central beta function* given by

$$\beta(p) \quad := \quad B(p,p) \;=\; \frac{\Gamma^2(p)}{\Gamma(2p)}$$

was needed to express $K[N]$. In every case $K[N]$ became products of beta functions and algebraic numbers only. In the cases of $N = 1,2$ (mod 4), only central beta functions were required. In these cases it was also found that β's always appeared in pairs of $\beta(p)\beta(\frac{1}{2}-p)$. So making use of the relation

$$\beta\left(\frac{1}{2}-p\right) = 2^{4p-1}\beta(p)\tan \pi p,$$

one could always reduce the argument of the $\beta(p)$'s involved so that $p \leq 1/4$.

One only really needs to give $K[N]$ for when N is square-free. Suppose that $N = n^2\mu$ where n and μ are positive integers, then it is known that

$$K[n^2\mu] \quad = \quad M_n(\mu)K[\mu],$$

where the *multiplier* $M_n(\mu)$ is *algebraic*. The following formulas for $M_n(\mu)$ are known:

$$\begin{aligned} M_2(\mu) &= \frac{1+k'_\mu}{2}, \\ 27M_3^4(\mu) - 18M_3^2(\mu) - 8(1-2k_\mu^2)M_3(\mu) - 1 &= 0, \\ (5M_5(\mu)-1)^5(1-M_5(\mu)) &= 256k_\mu^2(1-k_\mu^2)M_5(\mu). \end{aligned} \tag{9.22}$$

See [52], where many other multipliers are discussed.

These formulas for finding $K[4N]$, $K[9N]$, and $K[25N]$ from $K[N]$ depend only on knowing k_N. Thus, suppose that we wish to find $K[25]$ from $K[1]$. We substitute the value $k_1^2 = 1/2$ into (9.22). In this particular case (1.9) can be solved giving the result $M_5 = (\sqrt{5}+2)/5$, so $K[25] = (\sqrt{5}+2)K[1]/5$.

The list below gives $K[\mu]$ and if possible the value of k_μ^2 for $\mu = 1$ to 25. Many of these results were obtained using the *Mathematica* routine `Recognize` (or the *Maple* routine `identify`).

(a) Verify all the results below numerically. Then attempt to recover them knowing only the quantities K and n_N as defined above. Both *Maple* and *Mathematica* implement all the needed objects. In the table, R_1 denotes the real root of $t^3 - 4t - 4 = 0$, and R_2 denotes the root of $t^5 - 11(t-1)^2(t+1) = 0$ that is closest to one.

It will be seen that, for large N, $\tan(\pi n)$ is associated with each $\beta(n)$. Actually, this is so for every N that is expressed in terms of central β functions, but for small N the tangents can be found in terms of radicals. In fact, for $1 \le N \le 20$, excluding $N = 11$ and 19, all $K[N]$ can be expressed in quadratic surds and at most three central beta functions. The most surprising of these is perhaps the case $N = 17$—see below for details.

Following the first list is a second group of results, giving many higher values relying on the multipliers above. In this listing, R_3 is the real root of $1 - 2t + 4t^2 - 2t^3 = 0$ and R_4 is the root of $t^9 = 19(2t^7 - t^6 + 22t^5 + 19t^4 - 57t^3 - 19t^2 + 57t - 19)$.

(b) Likewise, attack the results in the second group of formulas numerically. Then attempt to recover them knowing only the quantities K and n_N as defined above and in some cases to simplify the given result.

$$K[1] = \frac{1}{4}\beta\left(\frac{1}{4}\right), \qquad k'^2_1 = \frac{1}{2};$$

$$K[2] = \frac{2^{3/4}}{16}\beta\left(\frac{1}{8}\right), \qquad k'^2_2 = 2(\sqrt{2}-1)^2;$$

$$K[3] = \frac{2^{1/3} \cdot 3^{1/4}}{12} \beta\left(\frac{1}{6}\right), \qquad k'^2_3 = \frac{2+\sqrt{3}}{4};$$

$$K[4] = \frac{(\sqrt{2}+2)}{16} \beta\left(\frac{1}{4}\right), \qquad k'^2_4 = 2^{\frac{5}{2}}(\sqrt{2}-1)^2;$$

$$K[5] = \frac{(42+19\sqrt{5}-2\sqrt{840+398\sqrt{5}})^{\frac{1}{4}}}{2^{\frac{12}{5}}5^{\frac{5}{8}}} \beta\left(\frac{1}{20}\right),$$
$$k'^2_5 = \frac{1+2\sqrt{\sqrt{5}-2)}}{2};$$

$$K[6] = \frac{2^{1/12} \cdot 3^{1/4}(\sqrt{2}-1)(\sqrt{3}+1)}{48} \beta\left(\frac{1}{24}\right),$$
$$k_6^2 = (\sqrt{3}-\sqrt{2})^2(2-\sqrt{3})^2;$$

$$K[7] = \frac{2^{5/7} \cdot 7^{3/4}}{14} \frac{\beta\left(\frac{1}{7}\right)\beta\left(\frac{2}{7}\right)}{\beta\left(\frac{1}{14}\right)}, \qquad k_7^2 = \frac{8-3\sqrt{7}}{16};$$

$$K[8] = \frac{2^{3/4}\left(1+\sqrt{2\sqrt{2}-2}\right)}{32} \beta\left(\frac{1}{8}\right), \qquad k_8^2 + \frac{1}{k_8^2} = 2(113+80\sqrt{2});$$

$$K[9] = \frac{(3+2\sqrt{3})^{1/2}}{12} \beta\left(\frac{1}{4}\right), \qquad k_9^2 = \frac{(2-\sqrt{3})(\sqrt{2}-3^{\frac{1}{4}})^2}{2};$$

$$K[10] = \frac{10^{1/4}(\sqrt{5}-2)^{1/2}}{80} \frac{\beta\left(\frac{1}{40}\right)\beta\left(\frac{9}{40}\right)}{\beta\left(\frac{3}{8}\right)},$$
$$k_{10}^2 = (\sqrt{10}-3)^2(\sqrt{2}-1)^4;$$

$$K[11] = \frac{R_1 R_2}{11^{\frac{3}{4}} 2^{\frac{29}{11}}} B\left(\frac{1}{22}, \frac{3}{22}\right),$$
$$16k_{11}^2(1-k_{11}^2) = 1 + \frac{4(21\sqrt{33}-27)^{\frac{1}{3}}}{3} - \frac{32}{(21\sqrt{33}-27)^{\frac{1}{3}}};$$

$$K[12] = \frac{2^{1/3} \cdot 3^{1/4}(\sqrt{6}+\sqrt{2}+4)}{96} \beta\left(\frac{1}{6}\right),$$
$$k_{12}^2 = (\sqrt{3}-\sqrt{2})^4(\sqrt{2}-1)^4;$$

$$K[13] = \frac{(5\sqrt{13}+18)^{1/4}}{13^{5/8}2^{29/13}} \sqrt{\sqrt{13}-1-\sqrt{13-2\sqrt{13}}} \, \frac{\beta\left(\frac{1}{52}\right)\beta\left(\frac{9}{52}\right)}{\beta\left(\frac{3}{52}\right)},$$
$$k_{13}^2 = \frac{1-6\sqrt{5\sqrt{13}-18}}{2};$$

$$K[14] = 2^{9/14}\cdot 7^{5/8}\left[\sqrt{2}(1+\sqrt{2\sqrt{2}+1})+\sqrt{2\sqrt{2}-1}\right]^{1/2}$$
$$\times \frac{(2\sqrt{2}-\sqrt{7})^{1/4}}{112\left[\frac{\beta\left(\frac{5}{56}\right)\beta\left(\frac{1}{8}\right)\beta\left(\frac{13}{56}\right)}{\beta\left(\frac{17}{56}\right)}\right]^{1/2}},$$
$$k_{14}^2 + \frac{1}{k_{14}^2} = 2\left[995+704\sqrt{2}+8\sqrt{14(2209+1562\sqrt{2})}\right];$$

$$K[15] = \frac{15^{1/4}(\sqrt{5}-1)}{60}\,\frac{\beta\left(\frac{1}{15}\right)\beta\left(\frac{4}{15}\right)}{\beta\left(\frac{1}{3}\right)},$$
$$k_{15}^2 = \frac{(2-\sqrt{3})^2(\sqrt{5}-\sqrt{3})^2(3-\sqrt{5})^2}{128};$$

$$K[16] = \frac{(\sqrt{2}+2^{1/4})^2}{32}\beta\left(\frac{1}{4}\right), \qquad k_{16}^2 = \frac{(\sqrt{2}-1)^4}{(2^{\frac{1}{4}}+1)^8};$$

$$K[17] = \frac{\left[5(\sqrt{17}+4)^{1/2}+6+2\sqrt{17}\right]^{\frac{1}{4}}}{2^{\frac{89}{34}}17^{\frac{9}{16}}}\left[\frac{\beta\left(\frac{1}{68}\right)\beta\left(\frac{9}{68}\right)\beta\left(\frac{13}{68}\right)}{\beta\left(\frac{15}{68}\right)}\right]^{\frac{1}{2}}$$
$$\times\left[\frac{\tan\left(\frac{\pi}{68}\right)\tan\left(\frac{9\pi}{68}\right)\tan\left(\frac{13\pi}{68}\right)}{\tan\left(\frac{15\pi}{68}\right)}\right]^{\frac{1}{4}},$$
$$k_{17}^2(1-k_{17}^2) = \frac{(u-\sqrt{u})^{12}}{2^{14}}, \qquad u = \frac{1+\sqrt{17}}{2}.$$

In investigating the group of tangents in the above formula, Zucker attempted to find the polynomial it satisfied, but was unsuccessful. Then almost by accident he tried

$$a = (\sqrt{17}+4)\left[\frac{\tan\left(\frac{\pi}{68}\right)\tan\left(\frac{9\pi}{68}\right)\tan\left(\frac{13\pi}{68}\right)}{\tan\left(\frac{15\pi}{68}\right)}\right]$$

and found it satisfied the degree-16 polynomial

$$\begin{aligned}
&t^{16}-1568t^{15}+812344t^{14}-152116064t^{13}+6117466780t^{12}\\
&+439568632160t^{11}-8244972920t^{10}-40944012640t^{9}\\
&-7384665274t^{8}+3230456480t^{7}+399961736t^{6}\\
&-63691040t^{5}-6458724t^{4}+306336t^{3}\\
&+28984t^{2}+480t+1=0.
\end{aligned}$$

This was found by evaluating a to 300 decimal places and using `Recognize` in *Mathematica*. Remembering Gauss and the 17-sided polygon, Zucker hoped this might be factored into quadratic factors, but this attempt was unsuccessful. He mentioned this to his colleague Richard Delves who, using *Maple*, factored the equation over various fields, as follows: First the degree-16 polynomial was factored into two degree-8 polynomials over the field $\sqrt{17}$. Then, with a hint from Rouse-Ball's book on recreational mathematics, the appropriate degree-8 factor that contained the correct root (determined numerically) was further factored into two degree-4 polynomials over the field $r_1 = \sqrt{34+2\sqrt{17}}$. The factor containing the required root was then factored into two quadratics over the field $r_2 = \sqrt{68+12\sqrt{17}-(7+\sqrt{17})r_1}$. On solving the relevant quadratic, one finds that

$$\begin{aligned}
a &= 98+24\sqrt{17}+\frac{3+\sqrt{17}}{8}r_1+\frac{9+2\sqrt{17}}{2}r_2\\
&\quad -\frac{3+\sqrt{17}}{16}r_1r_2-\frac{1}{4}\sqrt{b},
\end{aligned}$$

where

$$\begin{aligned}
b &= 64(6511+1579\sqrt{17})-8(1471+357\sqrt{17})r_1\\
&\quad +16(1681+408\sqrt{17})r_2-2(641+165\sqrt{17})r_1r_2.
\end{aligned}$$

One can thus express $K[17]$ as quadratic surds times central beta functions.

$$K[18]=\frac{2^{3/4}(\sqrt{6}+\sqrt{2}-1)}{48}\beta\left(\frac{1}{8}\right),$$
$$k_{18}^2=(2-\sqrt{3})^4(\sqrt{2}-1)^6;$$

$$K[19]=\frac{R_3R_4}{19^{\frac{3}{4}}2^{\frac{32}{19}}}\frac{B\left(\frac{1}{38},\frac{5}{38}\right)\beta\left(\frac{4}{19}\right)}{B\left(\frac{2}{19},\frac{4}{19}\right)},$$
$$16k_{19}^2(1-k_{19}^2)=1+12(3\sqrt{57}-1)^{\frac{1}{3}}-\frac{96}{(3\sqrt{57}-1)^{\frac{1}{3}}};$$

$$K[20] = \frac{1+k_5'}{2}K[5], \quad k_5'^2 = \frac{1+2(\sqrt{5}-2)^{1/2}}{2},$$
$$k_{20}^2 + \frac{1}{k_{20}^2} = 2\left[9873+4416\sqrt{5}+32\sqrt{5(38078+17029\sqrt{5})}\right];$$

$$K[21] = \frac{\left[2(2+\sqrt{3})(3+\sqrt{7})+\sqrt{7}\right]^{\frac{1}{4}}}{2^{\frac{52}{21}}(21)^{\frac{5}{8}}}\left[\frac{\beta\left(\frac{1}{84}\right)\beta\left(\frac{5}{84}\right)\beta\left(\frac{17}{84}\right)}{\beta\left(\frac{1}{4}\right)}\right]^{\frac{1}{2}}$$
$$\times\left[\tan\left(\frac{\pi}{84}\right)\tan\left(\frac{5\pi}{84}\right)\tan\left(\frac{17\pi}{84}\right)\right]^{\frac{1}{4}},$$
$$4k_{21}^2(1-k_{21}^2) = (8-3\sqrt{7})^2(3\sqrt{3}-2\sqrt{7})^2;$$

$$K[22] = \frac{\left[3\sqrt{22}+7+5\sqrt{2}\right]^{\frac{1}{2}}}{2^{\frac{137}{44}}\cdot 11^{\frac{3}{4}}}\left[\frac{\beta\left(\frac{1}{88}\right)\beta\left(\frac{9}{88}\right)\beta\left(\frac{19}{88}\right)}{\beta\left(\frac{5}{88}\right)\beta\left(\frac{7}{88}\right)}\right]$$
$$\times\left[\frac{\tan\left(\frac{\pi}{88}\right)\tan\left(\frac{9\pi}{88}\right)\tan\left(\frac{19\pi}{88}\right)}{\tan\left(\frac{5\pi}{88}\right)\tan\left(\frac{7\pi}{88}\right)}\right]^{\frac{1}{2}},$$
$$k_{22}^2 = (3\sqrt{11}-7\sqrt{2})^2(10-3\sqrt{11})^2;$$

$$K[24] = \frac{1+(\sqrt{3}-1)(\sqrt{2}+1)\sqrt{\sqrt{3}-\sqrt{2}}}{2}K[6],$$
$$k_{24}^2 = \left(\frac{1-u}{1+u}\right)^2, \quad u = (\sqrt{2}+1)(\sqrt{3}+1)\sqrt{\sqrt{3}-\sqrt{2}},$$
$$k_{24}^2 + \frac{1}{k_{24}^2} = 2\left[37745+21792\sqrt{3}+48\sqrt{2}(556+321\sqrt{3})\right];$$

$$K[25] = \frac{(\sqrt{5}+2)}{20}\beta\left(\frac{1}{4}\right), \qquad k_{25}^2 = \frac{(\sqrt{5}-2)^2(3-2\cdot 5^{\frac{1}{4}})^2}{2};$$

$$K[27] = \frac{3^{3/4}(2^{2/3}+2)^2}{216}\beta\left(\frac{1}{6}\right);$$

$$K[28] = \frac{8+3\sqrt{2}+\sqrt{14}}{16}K[7];$$

$$K[30] = \left(4+\sqrt{2}+2\sqrt{3}+\sqrt{5}+3\sqrt{6}+\sqrt{10}\right)^{\frac{1}{2}}$$
$$\times\left(\frac{49-20\sqrt{3}-16\sqrt{5}+12\sqrt{15}+2\sqrt{1760-970\sqrt{3}-752\sqrt{5}+454\sqrt{15}}}{2^{\frac{199}{15}}3^3\,5^2}\right)^{\frac{1}{4}}$$
$$\times\left[\frac{\beta\left(\frac{1}{120}\right)\beta\left(\frac{11}{120}\right)\beta\left(\frac{17}{120}\right)}{\beta\left(\frac{7}{120}\right)}\right]^{\frac{1}{2}},$$
$$k_{30}' = \sqrt{2\left(\sqrt{a^2+a}-a\right)}, \qquad a=(3+\sqrt{10})^4(2+\sqrt{5})^4;$$

$$K[32] = \frac{2^{\frac{3}{4}}}{64}\left\{1+\left[2(\sqrt{2}-1)\right]^{\frac{1}{4}}\right\}^2\beta\left(\frac{1}{8}\right);$$

$$K[33] = \frac{(3+\sqrt{11})^{\frac{1}{2}}(\sqrt{3}+1)^{\frac{3}{2}}(2\sqrt{3}-\sqrt{11})^{\frac{1}{4}}}{2^{\frac{227}{66}}33^{\frac{5}{8}}}$$
$$\times\left[\frac{\beta\left(\frac{1}{132}\right)\beta\left(\frac{17}{132}\right)\beta\left(\frac{25}{132}\right)\beta\left(\frac{29}{132}\right)}{\beta\left(\frac{31}{132}\right)\beta\left(\frac{1}{4}\right)}\right]^{\frac{1}{2}}$$
$$\times\left[\frac{\tan\left(\frac{\pi}{132}\right)\tan\left(\frac{17\pi}{132}\right)\tan\left(\frac{25\pi}{132}\right)\tan\left(\frac{29\pi}{132}\right)}{\tan\left(\frac{31\pi}{132}\right)}\right]^{\frac{1}{4}};$$

$$K[36] = \frac{3^{1/4}\sqrt{2}\left(1+\sqrt{2}+\sqrt{3}+3^{1/4}\right)}{48}\beta\left(\frac{1}{4}\right);$$

$$K[37] = \frac{(6+\sqrt{37})^{\frac{1}{2}}}{2^{\frac{72}{37}}\cdot 37^{\frac{5}{8}}}\left[\frac{\beta\left(\frac{1}{148}\right)\beta\left(\frac{9}{148}\right)\beta\left(\frac{21}{148}\right)\beta\left(\frac{25}{148}\right)\beta\left(\frac{33}{148}\right)}{\beta\left(\frac{3}{148}\right)\beta\left(\frac{7}{148}\right)\beta\left(\frac{11}{148}\right)\beta\left(\frac{27}{148}\right)}\right]$$
$$\times\left[\frac{\tan\left(\frac{\pi}{148}\right)\tan\left(\frac{9\pi}{148}\right)\tan\left(\frac{21\pi}{148}\right)\tan\left(\frac{25\pi}{148}\right)\tan\left(\frac{33\pi}{148}\right)}{\tan\left(\frac{3\pi}{148}\right)\tan\left(\frac{7\pi}{148}\right)\tan\left(\frac{11\pi}{148}\right)\tan\left(\frac{27\pi}{148}\right)}\right]^{\frac{1}{2}};$$

$$K[40] = \frac{1+\sqrt{2(2+\sqrt{5})^3(3\sqrt{2}-\sqrt{5}-2)}}{2}K[10];$$

$$K[42] = \frac{\sqrt{4(6+4\sqrt{2}+\sqrt{7}+\sqrt{12\left(17+5\sqrt{2}+5\sqrt{7}+\sqrt{14}\right)}}}{2^{\frac{17}{4}}3^{\frac{3}{4}}7^{\frac{1}{2}}}$$

$$\times \left[\frac{\beta\left(\frac{1}{168}\right)\beta\left(\frac{17}{168}\right)\beta\left(\frac{25}{168}\right)\beta\left(\frac{41}{168}\right)}{\beta\left(\frac{5}{168}\right)\beta\left(\frac{37}{168}\right)}\right]^{\frac{1}{2}}$$

$$\times \left[\frac{\tan\left(\frac{\pi}{168}\right)\tan\left(\frac{17\pi}{168}\right)\tan\left(\frac{25\pi}{168}\right)\tan\left(\frac{41\pi}{168}\right)}{\tan\left(\frac{5\pi}{168}\right)\tan\left(\frac{37\pi}{168}\right)}\right]^{\frac{1}{4}},$$

$$k'_{42} = \sqrt{\frac{-a+\sqrt{a^2+8a}}{4}}, \qquad a = (\sqrt{8}+\sqrt{7})^4(23+5\sqrt{21})^3;$$

$$K[44] = \frac{1}{24}\left[12-3\sqrt{2}+\sqrt{22}+\frac{8}{c}+2c\right]K[11],$$

$$c = 2^{\frac{1}{6}}\left(27-15\sqrt{3}+5\sqrt{11}-3\sqrt{33}\right)^{\frac{1}{3}};$$

$$K[45] = \frac{\sqrt{6}\left[\sqrt{(\sqrt{5}-1)}+\sqrt{3(\sqrt{5}+1)}\right]}{6}K[5];$$

$$K[48] = \frac{1+(\sqrt{2}-1)(\sqrt{3}-\sqrt{2})(\sqrt{6}+\sqrt{2})^{\frac{3}{2}}}{2}K[12];$$

$$K[49] = \frac{\sqrt{7+4\sqrt{7}+7^{1/4}\sqrt{2}(5+\sqrt{7})}}{28}\beta\left(\frac{1}{4}\right);$$

$$K[52] = \frac{1}{4}\left(\frac{2\sqrt{2}+5-\sqrt{13}}{\sqrt{2}}+\sqrt{5\sqrt{13}-17}\right)K[13];$$

$$K[54] = \frac{1}{9}\left\{3+3\sqrt{2}-2\sqrt{3}-\sqrt{5}+2\left[3\left(a+b\right)\right]^{1/3}+2\left[3\left(a-b\right)\right]^{1/3}\right\}$$
$$\times K[6],$$
$$a = -81-54\sqrt{2}+47\sqrt{3}+32\sqrt{6},$$
$$b = 3\sqrt{6(750+530\sqrt{2}-433\sqrt{3}-306\sqrt{6})};$$

$$K[56] = \frac{1+k'_{14}}{2}K[14];$$

$$K[57] = \frac{(\sqrt{3}+1)^{\frac{3}{2}}(13+3\sqrt{19})^{\frac{1}{2}}(2\sqrt{19}-5\sqrt{3})^{\frac{1}{4}}}{2^{\frac{127}{38}}\cdot 57^{\frac{5}{8}}}$$
$$\times\left[\frac{\beta\left(\frac{1}{228}\right)\beta\left(\frac{25}{228}\right)\beta\left(\frac{29}{228}\right)\beta\left(\frac{41}{228}\right)\beta\left(\frac{49}{228}\right)\beta\left(\frac{53}{228}\right)}{\beta\left(\frac{7}{228}\right)\beta\left(\frac{43}{228}\right)\beta\left(\frac{55}{228}\right)\beta\left(\frac{1}{4}\right)}\right]$$
$$\times\left[\frac{\tan\left(\frac{\pi}{228}\right)\tan\left(\frac{25\pi}{228}\right)\tan\left(\frac{29\pi}{228}\right)\tan\left(\frac{41\pi}{228}\right)\tan\left(\frac{49\pi}{228}\right)\tan\left(\frac{53\pi}{228}\right)}{\tan\left(\frac{7\pi}{228}\right)\tan\left(\frac{43\pi}{228}\right)\tan\left(\frac{55\pi}{228}\right)}\right]^{\frac{1}{2}};$$

$$K[58] = \frac{2^{-\frac{1}{58}}58^{\frac{1}{4}}\sqrt{70+99\sqrt{2}+13\sqrt{29}}}{232}$$
$$\times\left[\frac{\beta\left(\frac{1}{232}\right)\beta\left(\frac{9}{232}\right)\beta\left(\frac{25}{232}\right)\beta\left(\frac{33}{232}\right)\beta\left(\frac{35}{232}\right)\beta\left(\frac{49}{232}\right)\beta\left(\frac{51}{232}\right)\beta\left(\frac{57}{232}\right)}{\beta\left(\frac{5}{232}\right)\beta\left(\frac{7}{232}\right)\beta\left(\frac{13}{232}\right)\beta\left(\frac{23}{232}\right)\beta\left(\frac{29}{232}\right)\beta\left(\frac{45}{232}\right)\beta\left(\frac{53}{232}\right)}\right]$$
$$\times\left[\frac{\tan\left(\frac{1}{232}\right)\tan\left(\frac{9}{232}\right)\tan\left(\frac{25}{232}\right)\tan\left(\frac{33}{232}\right)\tan\left(\frac{35}{232}\right)\tan\left(\frac{49}{232}\right)\tan\left(\frac{51}{232}\right)\tan\left(\frac{57}{232}\right)}{\tan\left(\frac{5}{232}\right)\tan\left(\frac{7}{232}\right)\tan\left(\frac{13}{232}\right)\tan\left(\frac{23}{232}\right)\tan\left(\frac{29}{232}\right)\tan\left(\frac{45}{232}\right)\tan\left(\frac{53}{232}\right)}\right]^{\frac{1}{2}};$$

$$K[60] = \frac{16+\sqrt{2}(3-\sqrt{5})(2+\sqrt{3})(\sqrt{5}+\sqrt{3})}{32}K[15];$$

$$K[63] = \frac{\sqrt{3}+\sqrt{9+2\sqrt{21}}}{6}K[7];$$

$$K[64] = \frac{\sqrt{2}\left(2^{1/4}+1\right)^2+2^{17/8}\left(\sqrt{2}+1\right)^{1/2}}{64}\beta\left(\frac{1}{4}\right);$$

$$K[68] = \frac{1+k'_{17}}{2}K[17];$$

$$K[72] = \frac{1+(\sqrt{3}+\sqrt{2})^{\frac{3}{2}}(14\sqrt{2}-10-4\sqrt{6})^{\frac{1}{4}}}{2}K[18];$$

$$K[75] = \frac{1}{15}\left[5+2.10^{1/3}+(5+3\sqrt{5})10^{-1/3}\right]K[3];$$

$$K[76] = \frac{1}{24}\left[12-\sqrt{3}-\sqrt{38}+\frac{8(1+\sqrt{19})}{c}+2c\right]K[19],$$
$$c = \left(35\sqrt{2}+17\sqrt{38}+9\sqrt{6}+9\sqrt{114}\right)^{\frac{1}{3}};$$

$$K[80] = \frac{1+k'_{20}}{2} K[20];$$

$$K[81] = \frac{\left\{1+\left[2(1+\sqrt{3})\right]^{1/3}\right\}^2}{36} \beta\left(\frac{1}{4}\right);$$

$$K[84] = K[21]\left[\frac{\sqrt{21}+2\sqrt{7}-2\sqrt{3}+2\sqrt{2}-5}{4\sqrt{2}} + \frac{\sqrt{-41-24\sqrt{3}+16\sqrt{7}+9\sqrt{21}}}{4}\right];$$

$$K[88] = \frac{1+\sqrt{2(-19601-13860\sqrt{2}+5910\sqrt{11}+4179\sqrt{22}}}{2} K[22];$$

$$K[90] = K[10]\left[\frac{\sqrt{6}(\sqrt{2}-1)(\sqrt{5}-\sqrt{2}+1)}{6} + \frac{1}{3}\left(-45+33\sqrt{2}-54\sqrt{3}-21\sqrt{5}+39\sqrt{6} +15\sqrt{10}-24\sqrt{15}+17\sqrt{30}\right)^{1/2}\right];$$

$$K[96] = \frac{1+k'_{24}}{2} K[24];$$

$$K[98] = M_7(2)K[2];$$

$$K[99] = \sqrt{\frac{9+2(21\sqrt{33}-27)^{1/3}+2(54+6\sqrt{33})^{1/3}}{27}} K[11];$$

$$K[100] = \frac{4+2\sqrt{5}+\sqrt{2}(3+2\cdot 5^{1/4})}{80} \beta\left(\frac{1}{4}\right).$$

The simplest equation for the seventh order multiplier seems to be

$$7M_7(\mu) - \frac{1}{M_7(\mu)} = 6-16t+12t^2-8t^3, \text{ where } t^4 = k_\mu k_{49\mu}.$$

16. (Two Ramanujan-like identities for $1/\pi^2$ due to Zudilin.) While we indicated in Section 2.7 that there were very few formulas for $1/\pi^2$ of the exact form we sought, there are many other interesting related evaluations, including two recently noted by Zudilin [291]. The equality

$$u_n = \sum_{\nu=0}^{\infty} \frac{(\frac{1}{2})_\nu^3 (\frac{1}{2})_{n-\nu}}{\nu!^3 (n-\nu)!} = \sum_{\nu=0}^{\infty} \left(\frac{(\frac{1}{4})_\nu (\frac{3}{4})_{n-\nu}}{\nu!(n-\nu)!} \right)^2, \tag{9.23}$$

where $(a)_n = \Gamma(a+n)/\Gamma(a) = \prod_{k=0}^{n-1}(a+k)$, holds because both sides satisfy the recurrence relation

$$8(n+1)^3 u_{n+1} - (2n+1)(8n^2+8n+5)u_n + 8n^3 u_{n-1} = 0, \tag{9.24}$$

as proven in [291]. From this one can conclude (see [291] for proof):

Theorem 9.1. *Suppose that $|z| < 1$ and $|4z/(1-z)^2| < 1$, and let u_n be defined as in (9.23). Then the following identity holds:*

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^5 z^n}{n!^5} = \frac{1}{(1-z)^{1/2}} \sum_{n=0}^{\infty} \frac{u_n (\frac{1}{4})_n (\frac{3}{4})_n}{n!^2} \left(\frac{-4z}{(1-z)^2} \right)^n. \tag{9.25}$$

Now define the differential operator $\theta := z \cdot d/dz$, consider

$$\begin{aligned} g_1(z) &= 20\,\theta^2 f(z) + 8\,\theta f(z) + f(z), \\ g_2(z) &= 820\,\theta^2 f(z) + 180\,\theta f(z) + 13\, f(z), \end{aligned}$$

where $f(z)$ is given by (9.25), and substitute $z = -1/2^2$ and $z = -1/2^{10}$, respectively. Using the evaluations

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{(-1)^n (\frac{1}{2})_n^5 (20n^2+8n+1)}{n!^5 2^{2n}} &= \frac{8}{\pi^2}, \\ \sum_{n=0}^{\infty} \frac{(-1)^n (\frac{1}{2})_n^5 (820n^2+180n+13)}{n!^5 2^{10n}} &= \frac{128}{\pi^2}, \end{aligned}$$

which are proven in Section 3.1, and the formulas

$$\begin{aligned} \frac{(\frac{1}{4})_n (\frac{3}{4})_n}{n!^2} &= \frac{2^{-6n}(4n)!}{n!^2 (2n)!}, \\ u_n = \sum_{n=0}^{n} \frac{(\frac{1}{2})_k^3 (\frac{1}{2})_{n-k}}{k!^3 (n-k)!} &= 2^{-6n} \sum_{k=0}^{n} \binom{2k}{k}^3 \binom{2n-2k}{n-k} 2^{4(n-k)}, \end{aligned}$$

establish the following theorem:

Theorem 9.2. *The following identities are valid:*

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{U_n (4n)!(18n^2-10n-3)}{n!^2 (2n)! 2^{8n} 5^{2n}} &= \frac{10\sqrt{5}}{\pi^2}, \\ \sum_{n=0}^{\infty} \frac{U_n (4n)!(1046529n^2+227104n+16032)}{n!^2 (2n)! 5^{4n} 41^{2n}} &= \frac{5^4 41\sqrt{41}}{\pi^2}, \end{aligned}$$

where the sequence

$$U_n \quad := \quad \sum_{k=0}^{n} \binom{2k}{k}^3 \binom{2n-2k}{n-k} 2^{4(n-k)}$$

satisfies the recursion

$$(n+1)^3 U_{n+1} - 8(2n+1)(8n^2+8n+5)U_n + 4096n^3 U_{n-1} \quad = \quad 0.$$

See [88] and [292] for more discussion of like series for $1/\pi$ and $1/\pi^2$.

Exercises for Chapter 3

1. (A log-arctan integral.) The integral

$$\frac{2}{\sqrt{3}} \int_0^1 \log^8(x) \arctan[x\sqrt{3}/(x-2)] \frac{dx}{x+1}$$

satisfies a linear relation involving the constants $L_{-3}(10)$, $L_{-3}(9)\log 3$, $L_{-3}(8)\pi^2$, $L_{-3}(7)\zeta(3)$, $L_{-3}(6)\pi^4$, $L_{-3}(5)\zeta(5)$, $L_{-3}(4)\pi^4$, $L_{-3}(3)\zeta(7)$, $L_{-3}(2)\pi^8$, and $L_{-3}(1)\zeta(9)$, where $L_{-3}(s) = \sum_{n=1}^{\infty} [1/(3n-2)^s - 1/(3n-1)^s]$. Find the integer coefficients of this relation.

Check if this relation given extends to an analogous relation for the integral with $\log^{10} x$ in the numerator. How about for $\log^{12} x$?

2. (Sample integrals.) Evaluate the following integrals by numerically computing them and then trying to recognize the answers, either by using the Inverse Symbolic Calculator [84] or by using a PSLQ facility, such as that built into the Experimental Mathematician's Toolkit [15]. All of the answers are simple expressions involving familiar mathematical constants such as π, e, $\sqrt{2}$, $\sqrt{3}$, $\log 2$, $\zeta(3)$, G (Catalan's constant), and γ (the Euler-Mascheroni constant). Many of these can be evaluated analytically using symbolic computing software. The intent here is to provide exercises for numerical quadrature and constant recognition facilities.

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

   (b) $\int_0^\infty xe^{-x}\sqrt{1-e^{-2x}}\,dx$

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

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

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

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

   (g) $\int_0^{\pi/2} \frac{x^2\,dx}{\sin^2 x}$

   (h) $\int_0^{\pi/2} \log^2(\cos x)\,dx$

(i) $\int_0^1 \frac{\log^2 x\,dx}{x^2+x+1}$

(j) $\int_0^1 \frac{\log(1+x^2)\,dx}{x^2}$

(k) $\int_0^\infty \frac{\log(1+x^3)\,dx}{1-x+x^2}$

(l) $\int_0^\infty \frac{\log x\,dx}{\cosh^2 x}$

(m) $\int_0^1 \frac{\arctan x}{x\sqrt{1-x^2}}$

(n) $\int_0^{\pi/2} \sqrt{\tan t}\,dt$

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) $\pi\log 2$, (h) $\pi/2(\log^2 2+\pi^2/12)$, (i) $8\pi^3/(81\sqrt{3})$, (j) $\pi/2-\log 2$, (k) $2(\pi\log 3)/\sqrt{3}$, (l) $\log\pi - 2\log 2-\gamma$, (m) $[\pi\log(1+\sqrt{2})]/2$, (n) $\pi\sqrt{2}/2$.

3. (Sample infinite series.) Evaluate the following infinite series by numerically computing them and then trying to recognize the answers, either by using the Inverse Symbolic Calculator [84] or else by using a PSLQ facility, such as that built into the Experimental Mathematician's Toolkit [15]. All of the answers are simple expressions involving familiar mathematical constants such as π, e, $\sqrt{2}$, $\sqrt{3}$, $\log 2$, $\zeta(3)$, G (Catalan's constant), and γ (the Euler-Mascheroni constant).

   (a) $\sum_{n=0}^\infty \frac{50n-6}{2^n\binom{3n}{n}}$

   (b) $\sum_{n=0}^\infty \frac{2^{n+1}}{\binom{2n}{n}}$

   (c) $\sum_{n=0}^\infty \frac{12n2^{2n}}{\binom{4n}{2n}}$

   (d) $\sum_{n=0}^\infty \frac{(4n)!(1+8n)}{4^{4n}n!^4 3^{2n+1}}$

   (e) $\sum_{n=0}^\infty \frac{(4n)!(19+280n)}{4^{4n}n!^4 99^{2n+1}}$

   (f) $\sum_{n=0}^\infty \frac{(2n)!(3n)!4^n(4+33n)}{n!^5 108^n 125^n}$

   (g) $\sum_{n=0}^\infty \frac{(-27)^n(90n+177)}{16^n\binom{3n}{n}}$

   (h) $\sum_{n=0}^\infty \frac{275n-158}{2^n\binom{3n}{n}}$

   (i) $\sum_{n=1}^\infty \frac{8^n(520+6240n-430n^2)}{\binom{4n}{n}}$

   (j) $\sum_{n=1}^\infty \frac{\binom{2n}{n}}{n^2 4^n}$

   (k) $\sum_{n=1}^\infty \frac{(-1)^n}{n^3 2^n\binom{2n}{n}}$

   (l) $\sum_{n=0}^\infty \frac{8^n(338-245n)}{3^n\binom{3n}{n}}$

   (m) $\sum_{n=1}^\infty \frac{(-9)^n\binom{2n}{n}}{6n^2 64^n} - \sum_1^\infty \frac{3^n\binom{2n}{n}}{2n^2 16^n}$

Answers: (a) π, (b) $\pi+4$, (c) $3\pi+8$, (d) $2/(\pi\sqrt{3})$, (e) $2/(\pi\sqrt{11})$, (f) $15\sqrt{3}/(2\pi)$, (g) $120-64\log 2$, (h) $6\log 2-135$, (i) $-45\pi-1164$, (j) $\pi^2/6-2\log^2 2$, (k) $\log^3 2/6-\zeta(3)/4$, (l) $162-6\pi\sqrt{3}-18\log 3$, (m) $-\pi^2/18+\log^2 2-\log^2 3/6$.

These examples are due to Gregory and David Chudnovsky.

4. (AMM Problem 11148, April 2005.) Show that

$$\int_0^\infty \frac{(x^8-4x^6+9x^4-5x^2+1)\,dx}{x^{12}-10x^{10}+37x^8-42x^6+26x^4-8x^2+1} = \frac{\pi}{2}.$$

Solution.

(a) For convenience, first prove the following lemma.

Lemma 9.3. *Let C be a positively- oriented simple closed curve containing n distinct complex numbers $a_1,a_2,\ldots,a_n$.*
Let $Q(z) := \prod_{k=1}^n (z-a_k)$. Then

$$\int_C \frac{z^m}{Q(z)}\,dz = \begin{cases} 0, & m=0,1,\ldots,n-2; \\ 2\pi i, & m=n-1. \end{cases}$$

(b) Let I denote the integral. A partial fraction decomposition yields

$$\begin{aligned} I &= \int_0^\infty \left[\frac{(1+x)^2\,dx}{2(x^6+4x^5+3x^4+4x^3-2x^2-2x+1)} \right. \\ &\qquad \left. + \frac{(1-x)^2\,dx}{2(x^6-4x^5+3x^4-4x^3-2x^2+2x+1)}\right] \\ &= \int_{-\infty}^\infty \frac{(1-x)^2\,dx}{2(x^6-4x^5+3x^4-4x^3-2x^2+2x+1)} \\ &= \int_{-\infty}^\infty \frac{y^2\,dy}{2(y^6+2y^5-2y^4-4y^3+3y^2+4y+1)} \\ &= \int_{-\infty}^\infty \left[\frac{(-i-u+iu^2)\,du}{4(u^3+u^2+iu^2-2u+iu-1)} \right. \\ &\qquad \left. + \frac{(i-u-iu^2)\,du}{4(u^3+u^2-iu^2-2u-iu-1)}\right]. \end{aligned} \tag{9.26}$$

(c) Check that the roots of $u^3+u^2+iu^2-2u+iu-1$ are in the lower half-plane, while those of $u^3+u^2-iu^2-2u-iu-1$ (its complex conjugate) are in the upper half-plane. Denote these latter roots as $\{\alpha_k\}$, $k=1,\ldots,3$. Apply the lemma to (9.26) over a standard half-circle contour integral to get

$$I = 2\pi i\left(-\frac{i}{4}\right) = \frac{\pi}{2}.$$

All of this can be done entirely symbolically in a computer algebra system such as *Maple* or *Mathematica*—indeed this is how we discovered the basis for this proof. A generalization is straightforward.

5. Prove that

Theorem 9.4. *Let $q(x) = x^n + c_{n-1}x^{n-1} + \cdots + c_1 x + c_0$, $c_k \in \mathbb{C}$, be a polynomial whose roots all lie in the upper half-plane, and let $p(x) = -ix^{n-1} + d_{n-2}x^{n-2} + \cdots + d_1 x + d_0$, $d_k \in \mathbb{C}$. Then*

$$\int_{-\infty}^{\infty} \operatorname{Re}\left(\frac{p(x)}{q(x)}\right) = \pi.$$

Many variations are possible.

6. (AMM Problem 11113, November 2004.) Evaluate

$$I_k(a,b) \quad := \quad \int_0^{\infty}\int_0^{\infty} \frac{e^{-k\sqrt{x^2+y^2}} \sin(ax)\sin(by)}{\sqrt{x^2+y^2}\,xy}\, dx\, dy$$

in closed form for $a,b,k > 0$.

Solution. Since $I_k(a,b) = kI_1(a/k, b/k)$, as a simple change of variables shows, we study only $I(a,b) := I_1(a,b)$. The desired formula is

$$\begin{aligned} I(a,b) \quad = \quad & \frac{\pi b}{4}\log\left(b^2+1\right) + \frac{\pi a}{4}\log\left(a^2+1\right) \\ & -\frac{\pi b}{2}\log\left(\sqrt{a^2+1+b^2}-a\right) - \frac{\pi a}{2}\log\left(\sqrt{a^2+1+b^2}-b\right) \\ & -\frac{\pi}{2}\arctan\left(\frac{ab}{\sqrt{a^2+1+b^2}}\right). \end{aligned}$$

To prove this let

$$K(a,b) \quad := \quad \frac{d^2 I(a,b)}{da\, db}.$$

Then a change to polar variables produces

$$K(a,b) \quad = \quad \frac{\pi}{2\sqrt{1+a^2+b^2}}.$$

Finally a careful integration produces the formula.

Having found this formula, it is easier to confirm it by (symbolic) differentiation on observing that each term on the right vanishes when $a = 0$ or $b = 0$.

7. (Solution to AMM Problem 11152, May 2005.) Evaluate

$$\int_0^1 \frac{\log(\cos(\pi x/2))}{x(1+x)}\, dx.$$

Solution. The answer is $C := \log^2 2/2 - \log(2)\log(\pi)$. This value may be obtained immediately by placing a *Maple*-induced 50-digit approximation of the integral into the "Smart-Lookup" option of the Inverse Symbolic Calculator [84].

Let I denote the integral. We again need the dilogarithm function $\mathrm{Li}_2(x)$ and now use the easily provable identity

$$\mathrm{Li}_2 = -\int_0^x \log(1-z)/z\,dz.$$

Using the infinite product expansions for $\sin(x)$ and $\cos(x)$, we have

$$\begin{aligned}
I &= \int_0^1 \log(\cos(\pi x/2))/x\,dx - \int_1^2 \log(\sin(\pi x/2))/x\,dx \\
&= -\int_1^2 \log(\pi x/2)/x\,dx \\
&\quad + \sum_{k=1}^{\infty}\left[\int_0^1 \frac{1}{x}\log\left(1-\frac{x^2}{(2k-1)^2}\right)dx - \int_1^2 \frac{1}{x}\log\left(1-\frac{x^2}{4k^2}\right)dx\right] \\
&= C + \sum_{k=1}^{\infty}\left[\int_0^1 \frac{\log\left(1-\frac{x}{2k-1}\right)}{x}\,dx + \int_0^1 \frac{\log\left(1+\frac{x}{2k-1}\right)}{x}\,dx\right. \\
&\qquad \left. - \int_1^2 \frac{\log\left(1-\frac{x}{2k}\right)}{x}\,dx - \int_1^2 \frac{\log\left(1+\frac{x}{2k}\right)}{x}\,dx\right] \\
&= C + \sum_{k=1}^{\infty}\left[-\mathrm{Li}_2\left(\frac{1}{2k-1}\right) - \mathrm{Li}_2\left(-\frac{1}{2k-1}\right)\right. \\
&\qquad \left. + \mathrm{Li}_2\left(\frac{1}{k}\right) - \mathrm{Li}_2\left(\frac{1}{2k}\right) + \mathrm{Li}_2\left(-\frac{1}{k}\right) - \mathrm{Li}_2\left(-\frac{1}{2k}\right)\right] \\
&= C.
\end{aligned}$$

The last equality, a telescoping collapse, is justified since $\mathrm{Li}_2(x) = x + O(x^2)$ implies the sum is absolutely convergent.

Alternatively, one may rewrite the telescoping argument as a change of variables of the form

$$\int_1^2 \log(\cos(\pi x/2^N))/x\,dx = \int_{2^{-N}}^{2^{1-N}} \log(\cos(\pi t))/t\,dt.$$

8. (AMM Problem 11001, August-September 2004.) Evaluate

$$\int_0^{\infty} a\arctan\left(\frac{b}{\sqrt{a^2+x^2}}\right)\frac{1}{\sqrt{a^2+x^2}}\,dx \tag{9.27}$$

for $a, b > 0$.

Solution. An answer is

$$\begin{aligned}
&\int_0^{\infty} a\arctan\left(\frac{b}{\sqrt{a^2+x^2}}\right)\frac{1}{\sqrt{a^2+x^2}}\,dx \\
&\qquad = \frac{a\pi}{2}\left\{\log\left(b+\sqrt{a^2+b^2}\right) - \log(a)\right\}.
\end{aligned}$$

Indeed, making the two substitutions $x \to kt \to k\tan(s)$, where $k := a/b$, in (9.27) shows that it suffices to establish that

$$\int_0^{1/2\pi} \sec(s) \arctan\left(\frac{k}{\sec(s)}\right) ds = \frac{\pi}{2} \log\left(k + \sqrt{k^2+1}\right). \tag{9.28}$$

In turn, differentiation of (9.28) with respect to k yields

$$\frac{\pi}{\sqrt{1+k^2}} = \frac{\pi}{\sqrt{1+k^2}}.$$

Since both sides of (9.28) are zero when $k = 0$, an appeal to the fundamental theorem of calculus ends the argument.

9. (AMM Problem 11159, May 2005.) For $|a| < \pi/2$, evaluate in closed form

$$I(a) := \int_0^{\pi/2} \int_0^{\pi/2} \frac{\cos s\, ds\, dt}{\cos(a \cos s \cos t)}.$$

Hint: The series

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

wherein E_{2n} are the even *Euler numbers*, converges for $|x| < \pi/2$.

[The answer is $\pi/(2a) \log(\sec a + \tan a)$.]

Solution. (Due to David Bradley) Expand secant as a Maclaurin series in even powers of a:

$$\sec(a \cos\psi \cos\varphi) = \sum_{n=0}^{\infty} \frac{(-1)^n E_{2n}}{(2n)!} a^{2n} \cos^{2n}\psi \cos^{2n}\varphi. \tag{9.29}$$

Let $0 < r < 1$. We temporarily strengthen the restriction on a to $|a| \le r\pi/2$. The coefficients E_{2n} in (9.29) are the Euler numbers $1, -1, 5, -61, \ldots$ and satisfy an inequality of the form

$$\frac{|E_{2n}|}{(2n)!} < C\left(\frac{2}{\pi}\right)^{2n+1}, \qquad n \ge 0,$$

for C a constant independent of n (one can take $C = 2$). Thus, the series in (9.29) converges absolutely and uniformly in $[-r\pi/2, r\pi/2]$. Substitute into the integral and interchange summation and integration (as justified by uniform convergence) to get

$$I(a) = \sum_{n=0}^{\infty} \frac{(-1)^n E_{2n}}{(2n)!} a^{2n} \int_0^{\pi/2} \cos^{2n+1}\psi\, d\psi \int_0^{\pi/2} \cos^{2n}\varphi\, d\varphi.$$

In light of the known evaluations [149, 3.621]

$$\int_0^{\pi/2} \cos^{2n+1}\psi\, d\psi = \frac{2 \cdot 4 \cdots (2n)}{1 \cdot 3 \cdots (2n+1)}$$

and

$$\int_0^{\pi/2} \cos^{2n} \varphi \, d\varphi = \frac{1 \cdot 3 \cdots (2n-1)}{2 \cdot 4 \cdots (2n)} \frac{\pi}{2},$$

we have

$$I(a) = \frac{\pi}{2} \sum_{n=0}^{\infty} \frac{(-1)^n E_{2n}}{(2n)!} \frac{a^{2n}}{2n+1}.$$

Clearly $I(0) = \pi/2$. If $0 < |a| \le r\pi/2$, then interchange sum and integral again:

$$I(a) = \frac{\pi}{2a} \sum_{n=0}^{\infty} \frac{(-1)^n E_{2n}}{(2n)!} \int_0^a t^{2n} \, dt \tag{9.30}$$

$$= \frac{\pi}{2a} \int_0^a \sec t \, dt = \frac{\pi}{2a} \log(\sec a + \tan a). \tag{9.31}$$

Since $0 < r < 1$ is arbitrary, (9.31) is actually valid for $0 < |a| < \pi/2$.

What is perplexing here is that we need to know secant has a power series on $(-\pi/2, \pi/2)$ but nothing else!

10. (A sincing feeling.) Let

$$I_N := \int_0^{\infty} \prod_{n=0}^{N} \operatorname{sinc}\left(\frac{t}{2n+1}\right) dt. \tag{9.32}$$

   (a) Confirm both numerically and symbolically that each $I_N = \pi/2$ for $N < 7$, but $I_7 = 0.499999999992646859\,32\,\pi/2$. This occurs because $\sum_{n=1}^{6} 1/(2n+1) < 1 < \sum_{n=1}^{7} 1/(2n+1)$. (See [51].)

   (b) Now consider

$$J_N^1 := \int_0^{\infty} \prod_{n=0}^{N} \operatorname{sinc}\left(\frac{t}{3n+1}\right) dt$$

and

$$J_N^2 := \int_0^{\infty} \prod_{n=0}^{N} \operatorname{sinc}\left(\frac{t}{3n+2}\right) dt.$$

   Verify that $J_N^2 = \pi$ for $N < 5$ but not for $N = 5$, and relate this to the behavior of $\sum_{n=1}^{N} 1/(3n+2)$. See also Exercise 8 in Additional Exercises.

11. (Based on AMM Problem 11206.) Evaluate

$$\mathscr{L} := \lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} \left\{\frac{n}{k}\right\}^2.$$

Here $\{x\}$ denotes the fractional part of x.

Answer: $\mathscr{L} = \log(2\pi) - 1 - \gamma$.

Reason. Write $\mathscr{L}$ as a Riemann sum and change variables to obtain

$$\begin{aligned}\mathscr{L} &= \int_1^\infty \frac{\{x\}^2}{x^2}\,dx = \sum_{n=1}^\infty \int_0^1 \frac{x^2}{(x+n)^2}\,dx &(9.33)\\ &= 2\sum_{n=1}^\infty \left[1 - n\log\left(1+\frac{1}{n}\right) - \frac{1}{2\,(n+1)}\right]. &(9.34)\end{aligned}$$

Now use Abel summation and Stirling's approximation to obtain the claimed limit. Alternatively, use the series for log and rearrange to obtain

$$\mathscr{L} = 1 - 2\sum_{k=2}^\infty \frac{(-1)^k}{k+1}\,\zeta(k) = \log(2\pi) - 1 - \gamma,$$

where the last identity follows from [59, Equation (41)]. A third solution uses (9.33) and integrates by parts to write $\mathscr{L} = \int_0^1 x^2\,\Psi'(x+1)\,dx = 2\int_0^1 \log(\Gamma(x))\,dx - 1 - \gamma$. Now use the well-known evaluation

$$\int_0^1 \log\Gamma(x)\,dx = \log\sqrt{2\pi}, \tag{9.35}$$

given in Section 7.7.9. Working backwards gives another proof of this evaluation.

Note that one can recover the answer from PSLQ and (9.34) or (9.33) if one suspects the answer involves $\log(2), \log(\pi)$, and γ. Moreover, the *Inverse Calculator* recognizes the numerical value of the integral in (9.35).

One may make a similar analysis for

$$\mathscr{L}_f := \lim_{n\to\infty} \frac{1}{n}\sum_{k=1}^n f\left(\left\{\frac{n}{k}\right\}\right),$$

for more general functions f.

Exercises for Chapter 4

1. (Huygens' principle.) Sommerfeld states Huygens' Principle for the propagation of optical waves through some aperture as follows:

> *Light falling on the aperture propagates as if every [surface] element $[ds]$ emitted a spherical wave the amplitude and phase of which are given by that of the incident wave $[u^i]$* [257].

An analogous statement holds for scattering from obstacles, which we derive precisely here. Let Ω have C^2 boundary. We illuminate Ω with a plane wave $u^i(x,\widehat{\eta}) = e^{i\kappa\widehat{\eta}\cdot x}$. Suppose that the obstacle is *sound soft*, that is, the total field $u(x,\widehat{\eta}) = u^i(x,\widehat{\eta}) + u^s(x,\widehat{\eta}) = 0$ for $x \in \partial\Omega$. Show that

$$u^s(x,\widehat{\eta}) = -\int_{\partial\Omega} \frac{\partial u(y,\widehat{\eta})}{\partial\nu(y)}\Phi(x,y)ds(y), \quad x \in \Omega^o. \tag{9.36}$$

Interpret this in terms of Huygens' principle above.

Guide: Apply Green's formula (4.14) to the scattered field u^s (with justification for why you can do this), Green's theorem (4.13) to the incident field u^i, and use the boundary condition. Note that this argument does not make use of the explicit designation of the incident field, thus the statement (9.36) can be more broadly applied to *any* entire incident field v^i.

2. (Far field reciprocity.) Suppose that the scatterer Ω generates a total field u satisfying Dirichlet boundary conditions: $u = 0$ on $\partial\Omega$. Prove the reciprocity relation for the far field given by (4.17).

   Guide: Following the elegant argument of Colton and Kress [98], use Green's Theorem (4.13), the Helmholtz equation for the incident and scattered waves (4.3), the radiation condition (4.8) for the scattered wave, and the boundary integral equation for the far field pattern (4.16) to show that

$$\beta\left(u^\infty(\widehat{x},\widehat{\eta}) - u^\infty(-\widehat{\eta},-\widehat{x})\right) = \int_{\partial\Omega}\left(u(\cdot,\widehat{\eta})\frac{\partial u(\cdot,-\widehat{x})}{\partial \nu} - u(\cdot,-\widehat{x})\frac{\partial u(\cdot,\widehat{\eta})}{\partial \nu}\right),$$

   where β, in the two-dimensional setting, is given by (4.10).

   Show that this implies (4.17) when u satisfies the boundary condition $u(\cdot,\widehat{\eta}) = 0$ on $\partial\Omega$ for all $\widehat{\eta} \in \mathbb{S}$.

3. (Resolvent kernel for the Dirichlet Laplacian.) In the proof of Theorem 4.5 we made use of the resolvent kernel for the Dirichlet Laplacian. This is the total field for scattering due to an incident point source:

$$w^i(x,z) \equiv \Phi(x,z), \qquad x,z \in \mathbb{R}^2,\ x \neq z, \tag{9.37}$$

   where Φ is defined by (4.15). The total field satisfies the boundary value problem

$$\begin{aligned} (\triangle + \kappa^2)w(x,z) &= -\delta(x-z), \qquad x,z \in \Omega^o, \\ w(x,z) &= 0, \qquad x \in \partial\Omega. \end{aligned} \tag{9.38}$$

   Problem (9.38) is uniquely solvable [98] with $w = w^i + w^s$ for the scattered field w^s satisfying (4.8).

   Show that

$$w^s(x,z) = -\int_{\partial\Omega}\frac{\partial w(y,z)}{\partial \nu(y)}\Phi(x,y)\,ds(y), \quad x,z \in \Omega^o, \tag{9.39}$$

   analogous to (9.36).

4. (Symmetry of the resolvent kernel.) Continuing with the previous problem, show that the incident field w^i is spatially symmetric,

$$w^i(x,z) = w^i(z,x), \tag{9.40}$$

   thus w^s and w also have this property.

5. (Asymptotic behavior.) Let w satisfy (9.38) in Ω^o and $w = w^i + w^s$ with the incident point source $w^i(x,z) = \Phi(x,z)$. Let $u(z,-\widehat{x})$ be the total field from scattering due to the incident plane wave $u^i(z,-\widehat{x}) = e^{-i\kappa\widehat{x}\cdot z}$ with $u(z,-\widehat{x}) = 0$ on $\partial\Omega$. For β given by (4.10), show that the following relation holds as $|x| \to \infty$:

$$w(x,z) = \frac{e^{i\kappa|x|}}{|x|^{1/2}} \left\{ \beta u(z,-\widehat{x}) + O\left(|x|^{-1}\right) \right\}. \tag{9.41}$$

6. (Mixed reciprocity.) Use (9.41), together with the asymptotic behavior of a radiating solution to the Helmholtz equation given by (4.9) to show the mixed reciprocity relation:

$$w^\infty(\widehat{x},z) \;=\; \beta u^s(z,-\widehat{x}), \qquad \widehat{x} \in \mathbb{S},\; z \in \Omega^o, \tag{9.42}$$

for β given by (4.10).

7. (Potential theory.) In this exercise we use potential theoretic techniques to calculate the solution to the exterior Dirichlet problem, that is, u^s satisfying (4.3) on Ω^o with the boundary condition $u^s = f$ on $\partial\Omega$ and the radiation condition (4.8). To do this, we introduce the *acoustic single-* and *double-layer operators* given respectively as

$$\begin{aligned} (S\varphi)(x) &\equiv 2\int_{\partial\Omega} \varphi(y)\Phi(x,y)\, ds(y), \quad x \in \partial\Omega, \\ (K\varphi)(x) &\equiv 2\int_{\partial\Omega} \varphi(y)\frac{\partial\Phi(x,y)}{\partial\nu(y)}\, ds(y), \quad x \in \partial\Omega, \end{aligned} \tag{9.43}$$

where Φ is the two-dimensional fundamental solution given by (4.15). It can be shown [98] that, if the potential φ satisfies the integral equation

$$(I + K - i\gamma S)\varphi = f, \qquad \gamma \neq 0, \tag{9.44}$$

then u^s satisfies the exterior Dirichlet problem where u is given explicitly by

$$u(x) = \int_{\partial\Omega} \left(\frac{\partial\Phi(x,y)}{\partial\nu(y)} - i\gamma\Phi(x,y) \right) \varphi(y)\, ds(y), \quad x \in \mathbb{R}^2 \setminus \partial\Omega. \tag{9.45}$$

Show that the far field pattern due to scattering from a sound soft obstacle with an incident plane wave of direction $\widehat{\eta}$ is given by

$$u^\infty(\widehat{x},\widehat{\eta}) = \beta \int_{\partial\Omega} \left(\frac{\partial e^{-i\kappa\widehat{x}\cdot y}}{\partial\nu(y)} - ie^{-i\kappa\widehat{x}\cdot y} \right) \varphi(y)\, ds(y), \quad \widehat{x} \in \mathbb{S}, \tag{9.46}$$

where φ satisfies

$$(I + K - iS)\varphi = -e^{i\kappa x\cdot\widehat{\eta}}. \tag{9.47}$$

8. (Compute the far field pattern.) In this exercise, you will write a computer program to generate the far field data for scattering from the sound soft, kite-shaped obstacle shown in Figure 9.1 whose boundary is given parametrically by

$$\partial\Omega(\theta) \equiv (\cos\theta + 0.65\cos(2\theta) - 0.65, 1.5\sin\theta). \tag{9.48}$$

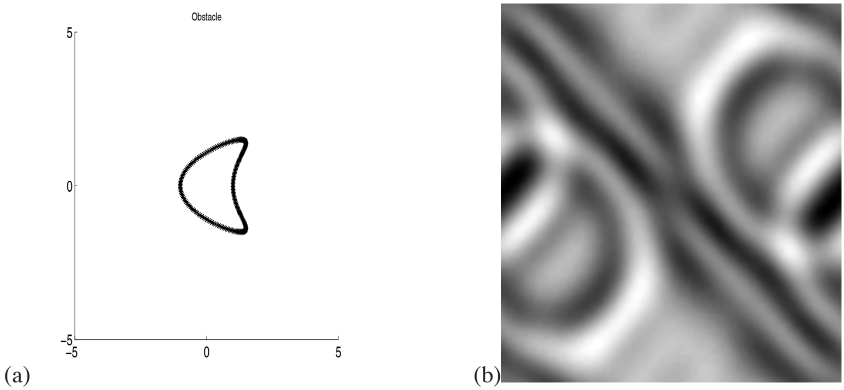


Figure 9.1. (a) Kite-shaped obstacle given by (9.48) and generated by the *Matlab* code in Section 4.5.1. (b) Real part of far field data for Exercise 8. Partial code for generating this data is given in Section 4.5.2.

We give the *Matlab* code (also runs with *Scilab*) to generate the obstacle and its normal derivative in Section 4.5.1 of Chapter 4.

Use (9.46)–(9.47) to calculate the far field data at 128 points equally distributed on $[-\pi, \pi]$ (full aperture) for a wavelength $\kappa = 3$ and 128 incident field directions $\widehat{\eta}$ coincident with the far field "measurement" points. Your answer should have real part resembling Figure 9.1(b). As a guide, we give in Section 4.5.2 a partial *Matlab* code (also runs in *Scilab*) to generate the far field data.

9. (Is the scatterer absorbing?) Show either numerically or analytically that the singular values of the far field operator $\mathscr{A}$ corresponding to the data in Exercise 8 lie on the circle centered at $\frac{1}{2\kappa}\left(\Im(\beta^{-1}), \Re(\beta^{-1})\right)$ and passing through the origin, hence the scatterer, as we already know, is nonabsorbing.

10. (Linear sampling.) At each point z_j corresponding to a sample point on a rectangular grid in the computational domain $[-5,5] \times [-5,5]$, compute the density g_{z_j} that satisfies the unconstrained, Tikhonov-regularized optimization problem

$$\underset{g \in \mathbb{C}^n}{\text{minimize}} \ \|\mathscr{A} g - \Phi^\infty(z_j, \cdot)\|^2 + \alpha \|g\|^2,$$

where $\mathscr{A}$ is the discrete far field operator generated from the data computed in Exercise 8 and the regularization parameter $\alpha \approx 1e-7$. Generate a surface plot of the value $\|g_j\|$ versus z_j. If you choose the dynamic range of your surface plot correctly, you should see something with a hole resembling the kite shown in Figure 9.1(a).

Hint: The solution to the optimization problem can be written in closed form via the normal equations (see Chapter 4, (4.43)).

Exercises for Chapter 5

1. (The Takagi function for $0 < a < \frac{1}{2}$.) Discuss and prove the differentiability properties of the Takagi function $T_{a,2}$ for $0 < a < \frac{1}{2}$.
   Hint: It is relatively easy to conjecture that, for $a < \frac{1}{2}$, $T_{a,2}$ does *not* have a derivative at any dyadic rational, but is differentiable everywhere else. This conjecture, however, is only "almost" true: There is precisely one exceptional value of a strictly between 0 and $\frac{1}{2}$ for which the conjecture is wrong. What is this value?
2. (Differentiability of the Weierstrass cosine series.) Prove that the Weierstrass cosine series $C_{a,2}$ for $1/2 \leq a < 1$ is nowhere differentiable.
3. (Singular functions.) Choose $0 < a < 1$. Discuss and prove the differentiability properties of the unique continuous solution of the system
   $$\begin{aligned} f\left(\frac{x}{2}\right) &= a f(x) \\ f\left(\frac{x+1}{2}\right) &= (1-a) f(x) + a \end{aligned}$$
   on $[0,1]$.
   Hint: Except for $a = \frac{1}{2}$, the function is *singular* (i.e., strictly monotone, with $f'(x) = 0$ a.e.). This example is from [115].
4. (The Cantor function.) Show that the system of functional equations
   $$\begin{aligned} f\left(\frac{x}{3}\right) &= \frac{1}{2} f(x) \\ f\left(\frac{x+1}{3}\right) &= \frac{1}{2} \\ f\left(\frac{x+2}{3}\right) &= \frac{1}{2} f(x) + \frac{1}{2} \end{aligned}$$
   on $[0,1]$ has a unique continuous solution, and discuss its differentiability properties.
   Hint: The solution is a (the) *Cantor function*. In general, we call an $f : [0,1] \to [0,1]$ a Cantor function if it is surjective but constant on each of a collection of intervals which together have full measure (such as the complement of the Cantor set). This example is from [252].
5. (One-sided differentiability.) Prove the following sharper version of Theorem 5.2: *Assume that* $f \in C[0,1]$ *has a finite one-sided derivative at some point in* $[0,1]$. *Then*
   $$\lim_{n\to\infty} 2^n \cdot \min\left\{\left|\gamma_{i,n}(f)\right| : i = 0, \ldots, 2^{n-1} - 1\right\} = 0.$$
6. (The Minkowski function.) Minkowski's ?-function is defined as follows. Let $x \in [0,1)$ with simple continued fraction $[0; a_1, a_2, a_3, \ldots]$. Then
   $$?(x) := \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{2^{a_1+\cdots+a_k-1}}.$$

This function maps the rational numbers onto the dyadic rationals and the quadratic irrationals onto the rationals.

Find a system of functional equations that characterizes the Minkowski function and then use the functional equations to derive its differentiability properties.

7. (The Riemann function.) The function

$$R(x) := \sum_{n=1}^{\infty} \frac{\sin(n^2 \pi x)}{n^2}$$

was apparently communicated by Riemann to his pupils as an example of a function that does not have a finite derivative at a dense set of points [121,158]. This function is, in fact, nondifferentiable almost everywhere, but it does have finite derivatives at certain rational values, which in turn form a dense set [141,142].

Find a basis suitable for analyzing this function.

8. (A binary recursion.)

(a) Let $x \geq 0$. Set $a_0 = x$ and

$$a_{n+1} = \frac{2a_n}{1-a_n^2} \quad (\text{with } a_{n+1} = -\infty \text{ if } a_n = \pm 1).$$

Prove that

$$\sum_{\substack{a_n<0\\ n\geq 0}} \frac{1}{2^{n+1}} = \frac{\arctan x}{\pi}.$$

(b) In general (see also [67]), let an interval $I \subseteq \mathbb{R}$ and subsets $D_0, D_1 \subseteq I$ with $D_0 \cup D_1 = I$ and $D_0 \cap D_1 = \emptyset$ be given, as well as functions $r_0 : D_0 \to I$, $r_1 : D_1 \to I$. Then consider the system (S) of the following two functional equations for an unknown function $f : I \to [0,1]$:

$$2f(x) = f(r_0(x)) \quad \text{if } x \in D_0, \tag{S_0}$$

$$2f(x) - 1 = f(r_1(x)) \quad \text{if } x \in D_1. \tag{S_1}$$

Such a system always leads to an iteration:

$$a_0 = x \quad \text{and} \quad a_{n+1} = \begin{cases} r_0(a_n), & a_n \in D_0; \\ r_1(a_n), & a_n \in D_1. \end{cases}$$

Prove that

$$f(a_0) = f(x) = \sum_{\substack{a_n \in D_1\\ n\geq 0}} \frac{1}{2^{n+1}}.$$

(c) Find parameters such that the following functions can be written as solutions of the system (S) and thus can be computed via their binary expansion: $\log(x)/\log(2)$ on $[1,2]$, $\arccos(x)/\pi$ on $[-1,1]$, and

$$\left\{ \begin{matrix} \arctan(x)/\pi, & x \in [0,\infty) \\ 1+\arctan(x)/\pi, & x \in (-\infty,0) \end{matrix} \right\}$$

.

(d) Find parameters such that a singular function or a Cantor function is a solution of (S).

(e) Experiment by plotting the solution for arbitrary (or intelligent) choices of the parameters.

9. (The Schilling equation.) The Schilling equation is the functional equation

$$4q\,f(qt) \;=\; f(t+1)+2f(t)+f(t-1) \quad \text{for } t\in\mathbb{R}$$

with a parameter $q\in(0,1)$. It has its origin in physics, and although it has been studied intensively in recent years, there are still many open questions connected with it. The main question is to find values of q for which the Schilling equation has a nontrivial L^1-solution. Discuss this question.

Hint: If an L^1-function f satisfies (5.9), then a rescaled version of $f*f$ satisfies the Schilling equation.

10. (Unboundedness of the iteration.) Is the sequence of iterates $B_q^n f^{(0)}$ unbounded for $q=(\sqrt{5}-1)/2$ (or any other Pisot or non-Pisot q) and for, say,

$$f^{(0)} = \frac{1-q}{2}\,\chi_{[-\frac{1}{(1-q)},\frac{1}{(1-q)}]}?$$

11. (Plotting f_q.) Find a good algorithm for computing and plotting the iterates $B_q^n f^{(0)}$ or any other approximation to f_q, for arbitrary q.

Exercises for Chapter 6

Some of the following exercises are relatively straightforward; others are open-ended and could be used as the starting point for an experimental research project.

1. Use Kraitchik's method to factorize 2041.

2. Find an n for which Kraitchik's method works, but we don't get an easy factorization via Fermat's method.

3. Rediscover the diagonalization of the $(k+1)\times(k+1)$ matrix T

$$T_{ij} = \frac{\binom{i}{\frac{w+i-j}{2}}\binom{k-i}{\frac{w-i+j}{2}}}{\binom{k}{w}}$$

by computing explicit examples in *Maple* or *Mathematica*: Use Sloane's database to help identify sequences.

4. Investigate the eigenstructure of other structured matrices: For example, consider the Toeplitz matrices

$$T_n = \begin{pmatrix} 1 & 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 1 & 0 & \dots & 0 \\ 0 & 1 & 1 & 1 & \dots & 0 \\ 0 & 0 & 1 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & & & & & 1 \end{pmatrix}.$$

Compute the eigenvalues for various values of n, plotting the values in increasing order. Guess, with the help of the Inverse Symbolic Calculator if necessary, a formula for the jth largest eigenvalue of T_n. Compute the corresponding eigenvectors, and guess the formula for their entries. For more information on this and related problems, see Doust, Hirshhorn, and Ho [120].

5. Fix the dimension k of the vector space, and find a way of uniformly generating binary vectors of weight 3. For various values of k, generate random vectors until you obtain a linearly dependent set. Compare the number of vectors required to the upper and lower bounds given above. Do you think that there is a sharp threshold?

6. When $\mathscr{P}$ is the set of primes congruent to 1 (mod 4), what are the values of the constants δ and K appearing in Wirsing's theorem?

7. Pick a moderately large value n (the product of two large primes would be appropriate). Using *Maple* or *Mathematica*, estimate the constants δ and K appearing in Wirsing's theorem.

8. For those who know about quadratic reciprocity: Suppose that n is the product $n = q_1 q_2$ of two primes. Find a condition *on* p for a prime p to be such that n is a quadratic residue $(\text{mod } p)$. Assuming Dirichlet's theorem (that if a and m are relatively prime then the number of primes congruent to $a \pmod{m}$ is asymptotic to $1/\phi(m)$), deduce that the relative density of $\mathscr{P}$ in the set of all primes should be $1/2$. Compare the value of δ from the previous exercise to 1/2.

9. For small y, compare the value of $Z_{\mathscr{P}}(y)$ to the value predicted (for *large* y) by Wirsing's theorem. Does our assumption that $Z_{\mathscr{P}}(y)$ behaves similarly for small and for large y seem justified?

10. Devise some statistical tests to determine whether the heuristic that

$$\alpha_j = \Pr(p_j | x^2 - n) \simeq c \frac{\log(p_j)}{p_j}$$

is a reasonable one. For example, the number $x^2 - n$ lies between $\sqrt{n}$ and n, and so the sums

$$\frac{1}{2} \log n < \sum_{p_j | x^2 - n} \log p_j < \log n$$

and

$$\sum_{j=1}^{k} \alpha_j \log p_j$$

should be about the same. (This ignores primes dividing $x^2 - n$ to the second or higher power, but their effect is small.) Note that this heuristic illustrates again the fact that the size of $\mathscr{B}$ has an impact on the probability that a $\mathscr{B}$-smooth number is divisible by p.

11. Generate $l \times k$ random matrices with $\alpha_j = c/j$ for various values of c. Iteratively remove colons and solons from the array until all columns are either empty or have at least three 1's . If there are more nonzero rows than columns, then the rows of the original array are linearly dependent.

    (a) What is the runtime of the algorithm to delete all colons and solons?

    (b) How large should l be as a function of k so that the rows of the initial array are linearly dependent?

    (c) How large should l be as a function of k so that the final array has more nonzero rows than columns? Suggested values to try: $l = 0.5k$, $l = 0.6k$, $l = 0.9k$, and $l = k+1$.

    (d) How many nonzero rows and columns does the final array have?

12. Suppose that a column of A contains exactly three 1's and that A has X_1 solons. After deleting the solons, what is the probability that the column now contains two 1's?

13. Suppose that A has X_1 solons, X_2 colons, and X_3 columns with exactly three 1's. If we remove the colons and then the solons, the columns with exactly three 1's can remain unchanged or can become colons, solons, or empty. What is the expected number of each that will be produced?

14. Suppose that A has X_1 solons, X_2 colons, and X_r columns with exactly r 1's. If we remove the colons and then the solons, the columns with exactly r 1's can become columns with s 1's, $0 \le s \le r$. What is the expected number of each that will be produced?

15. Consider a stochastic model for the deletion of colons and solons along the following lines: Consider the random variable

$$X(t) = (X_0(t), X_1(t), X_2(t), \ldots),$$

where $X_i(t)$ is the number of columns containing exactly i 1's after t rounds of deletions of solons and colons. More precisely, $X(t-1)$ is the number before the tth round of deletions. In round t, remove all colons (by replacing colon-rows with their sum), and then remove all solons. Now update $X(t)$. Develop heuristics (by making reasonable assumptions where necessary) for the dynamics of $X(t)$.

16. Explain the seemingly paradoxical fact that increasing the number of columns in A *decreases* the size of the final nonzero array after iterated deletions. For example, the values in the following table are typical. Each row is the result of iterated deletions of solons and colons for a random array A with $\alpha_j = 0.72/j$. The final size is the number of nonzero rows and columns.

Initial size	Final size
10000×10000	4700×2300
10000×15000	2250×1300
10000×20000	800×480
10000×25000	300×180
10000×30000	150×100
10000×35000	100×50
10000×40000	47×22
10000×45000	38×20

17. (The continued fraction for e [93, 225] and [52, Theorem 11.1].) Consider the continued fraction
$$\mu := [1,0,1,1,2,1,1,4,1,1,6,1,8,1,...],$$
with convergents p_n, q_n. Define the following three integrals:
$$A_n := -\int_0^1 \frac{x^n (x-1)^n}{n!} e^x dx,$$
$$B_n := \int_0^1 \frac{x^{n+1} (x-1)^n}{n!} e^x dx,$$
$$C_n := \int_0^1 \frac{x^n (x-1)^{n+1}}{n!} e^x dx.$$
Verify, and then prove inductively, that $A_n = p_{3n} - q_{3n}e$, $B_n = p_{3n+1} - q_{3n+1}e$, and $C_n = p_{3n+2} - q_{3n+2}e$.

   (a) Deduce that $\mu = e$.

   (b) Generalize this argument to show that for any $M > 0$
   $$e^{1/M} = [1, M-1, 1, 1, 3M-1, 1, 1, , 1, 1, 5M-1, 1, 7M-1, 1, ...].$$
   In particular, since the (simple) continued fraction neither terminates nor repeats, for positive integer M, $\exp(1/M)$ is irrational.
   Hint: use $A_n := -\int_0^1 \frac{x^n (x-1)^n}{n!} e^{x/M} M^{-n-1} dx$.

Exercises for Chapter 7

1. Give a direct proof of Wallis' formula
$$\int_0^\infty \frac{dx}{(x^2+1)^{m+1}} = \frac{\pi}{2^{2m+1}} \binom{2m}{m}. \tag{9.49}$$

Hint: Convert the integral into a value of the beta function (7.75) and use the value $\Gamma(1/2) = \sqrt{\pi}$ that we discussed in Chapter 7 and that can also be obtained directly from *Mathematica* or be reduced to a well-known evaluation.

Generalize the previous argument to obtain the value

$$\int_0^\infty \frac{dx}{(x^4+1)^{m+1}} = \frac{\pi}{m!\,2^{2m+3/2}} \prod_{k=1}^{\infty}(4k-1). \tag{9.50}$$

2. In the evaluation of the quartic integral $N_{0,4}(0;m)$, one can prove by completely elementary means that the polynomial P_m in (7.77) is also given by

$$\begin{aligned} P_m(a) &= \sum_{j=0}^{m} \binom{2m+1}{2j} (a+1)^j \\ &\quad \times \sum_{k=0}^{m-j} \binom{m-j}{k} \binom{2(m-k)}{m-k} 2^{-3(m-k)} (a-1)^{m-k-j}. \end{aligned} \tag{9.51}$$

Prove that these two forms coincide.

Compute the value of $P_m(1)$ using both forms of P_m to produce

$$\sum_{k=0}^{m} 2^{-2k} \binom{2k}{k} \binom{2m-k}{m} = \sum_{k=0}^{m} 2^{-2k} \binom{2k}{k} \binom{2m+1}{2k}. \tag{9.52}$$

Mathematica converts this identity into

$$-\frac{2^{2m+1}\sqrt{\pi}}{\Gamma(-1/2-2m)\,\Gamma(2m+2)} = \frac{2^{2m+1}\,\Gamma(3/2+2m)}{\sqrt{\pi}\,\Gamma(2m+2)}. \tag{9.53}$$

Use elementary properties of the gamma function to check this directly.

Use the WZ-method to prove (9.52). Check that both sides satisfy the recursion

$$(2m+3)(2m+2)f(m+1) = (4m+5)(4m+3)f(m). \tag{9.54}$$

It would be interesting to provide a direct proof of (9.52).

3. The study of 2-adic properties of the coefficients appearing in the quartic integral requires an elementary fact of binomial coefficients:

Fact. The central binomial coefficient

$$C_m := \binom{2m}{m} \tag{9.55}$$

is even. Moreover $\frac{1}{2}C_m$ is odd if and only if m is a power of 2. This exercise outlines a new proof. The exact power of 2 that divides m is denoted by $\nu_2(m)$.

   (a) Prove that $m \geq \nu_2(m!)$.

   Hint: Use (7.88).

(b) Check that $\nu_2((2^n)!) = 2^n - 1$. Now, let a be the largest integer such that $m = 2^a + b$; then,

$$\nu_2(m!) = \nu_2((2^a)!) + \nu_2(b!). \tag{9.56}$$

(c) To conclude, check that

$$\nu_2(C_m) = 2^a + b - \nu_2((2^a+b)!) > 1. \tag{9.57}$$

4. The polynomial $2^{2m}P_m(a)$ has positive integer coefficients. It seems to have many interesting properties when considered modulo a prime p. Use a symbolic language to explore them. You can report your results to vhm@math.tulane.edu.

5. The integers

$$b_{l,m} \quad = \quad \sum_{k=l}^{m} 2^k \binom{2m-2k}{m-k}\binom{m+k}{m}\binom{k}{l} \tag{9.58}$$

appear in the polynomial P_m as

$$P_m(a) = 2^{-2m}\sum_{l=0}^{m} b_{l,m}a^l. \tag{9.59}$$

The sequence $\{b_{l,m} : 0 \leq l \leq m\}$ is known to be unimodal. See [40] for a proof. We have conjectured that this sequence is logconcave. Use the WZ-method to check that $b_{l,m}$ satisfies

$$b_{l+1,m} = \frac{2m+1}{l+1}b_{l,m} - \frac{(m+l)(m+1-l)}{l(l+1)}b_{l-1,m}. \tag{9.60}$$

Therefore, the sequence is logconcave provided that

$$(m+l)(m+1-l)b_{l-1,m}^2 + l(l+1)b_{l,m}^2 - l(2m+1)b_{l-1,m}b_{l,m} \geq 0. \tag{9.61}$$

Prove that the left-hand side attains its minimum at $l = m$ with value $2^{2m}m(m+1)\binom{2m}{m}^2$. *We cannot do this part.*

A generalization. The coefficients $\{b_{l,m}\}$ seem to have a property much stronger than logconcavity. Introduce the operator $\mathfrak{L}$ on the space of sequences, via

$$\mathfrak{L}(a_l) := a_l^2 - a_{l-1}a_{l+1}. \tag{9.62}$$

Therefore, $\{a_l\}$ is logconcave if $\mathfrak{L}(a_l)$ is nonnegative. We say that $\{a_l\}$ is r-logconcave if $\mathfrak{L}^{(k)}(a_l) \geq 0$ for $0 \leq k \leq r$. The sequence $\{a_l\}$ is ∞-logconcave if it is r-logconcave for every $r \in \mathbb{N}$.

Conjecture 9.5. *For each $m \in \mathbb{N}$, the sequence $\{b_{l,m} : 0 \leq l \leq m\}$ is ∞-logconcave.*

The binomial coefficients yield the canonical sequence on which these issues are tested. The solution of the next conjecture should provide guiding principles on how to approach Conjecture 9.5.

Conjecture 9.6. *For $m \in \mathbb{N}$ fixed, the sequence of binomial coefficients $\{\binom{m}{l}\}$ is ∞-logconcave.*

A direct calculation proves the existence of rational functions $R_r(m,l)$ such that

$$\mathfrak{L}^{(r)}\binom{m}{l} = \binom{m}{l}^{2^r} R_r(m,l). \tag{9.63}$$

Moreover, R_r satisfy the recurrence

$$R_{r+1}(m,l) = R_r^2(m,l) - \left[\frac{l(m-l)}{(l+1)(m-l+1)}\right]^{2^r} \times R_r(m,l-1)R_r(m,l+1).$$

Therefore, we *only* need to prove that $R_r(m,l) \geq 0$. This could be difficult.

6. The integral $N_{0,4}(a;m)$ appeared in a most intriguing expansion. The main result of [42] is that

$$\sqrt{a+\sqrt{1+c}} \quad = \quad \sqrt{a+1} + \frac{1}{\pi\sqrt{2}} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} N_{0,4}(a;k-1)c^k.$$

The proof employs Ramanujan's Master Theorem:

Theorem 9.7. *Suppose that F has a Taylor expansion around $c=0$ of the form*

$$F(c) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \varphi(k) c^k. \tag{9.64}$$

Then, the moments of F, defined by

$$M_n = \int_0^{\infty} c^{m-1} F(c)\, dc, \tag{9.65}$$

can be computed via $M_n = \Gamma(m)\varphi(-m)$.

Our expansion comes from the value

$$\int_0^{\infty} \frac{dx}{bx^4 + 2ax^2 + 1} = \frac{\pi}{2\sqrt{2}} \frac{1}{\sqrt{a+\sqrt{b}}}. \tag{9.66}$$

This explains the appearance of the double square root.

It would be interesting to provide a different type of proof. The reader should first use a symbolic language to find a closed-form expression for the coefficients in

$$\sqrt{b+\sqrt{a+\sqrt{1+c}}} = \sum_{k=0}^{\infty} \rho_k(a,b) c^k. \tag{9.67}$$

The polynomials

$$P_k^*(a,b) = b^k P_k\left(\frac{a}{b}\right) \tag{9.68}$$

will play a role in this expression. The polynomials $P_k^*(a,b)$ are the *homogenization* of $P_k(a)$.

7. Define the function

$$e_l(m) = \frac{(m-l)!l!m!}{(m+l)!2^m} b_{l,m}, \tag{9.69}$$

where $b_{l,m}$ are the integers defined in Exercise 5. Use the recurrence for $b_{l,m}$ to check that

$$Q_{m-j}(m) = e_{m-j}\left(\frac{m}{2}\right), \tag{9.70}$$

for j indepedent of m, is a polynomial in m. Confirm that Q_{m-j} is of degree j. For example, $Q_{m-3}(m) = m^3 + 2m + 3$. Compute the value of $Q_{m-j}(-1)$, and check that $m+1$ divides $Q_{m-j}(m)$ for j odd.

8. The function

$$\text{jump}_i(j) \quad = \quad \nu_2(i+j) - \nu_2(i), \quad i, j \in \mathbb{N}, \tag{9.71}$$

seems to appear in the description of the 2-adic values of the integers $b_{l,m}$ in Exercise 5. The index i is fixed, and the word *seems* is to be taken as "we have a conjecture, that we are not ready to make public." Use a symbolic language to generate interesting conjectures about jump_i.

9. The integral 4.351 of Gradshteyn and Rhyzik [149] states that

$$\int_0^1 (1-x)e^{-x} \log x \, dx = \frac{1-e}{e}. \tag{9.72}$$

Define the function

$$q_n \quad = \quad \int_0^1 x^n e^{-x} \log x \, dx + n! \left(\gamma + \Gamma(0,1)\right), \tag{9.73}$$

where $\Gamma(a,z)$ is the incomplete gamma function (8.26) and γ is the Euler-Mascheroni constant.

Explore the sequences of positive integers a_n, b_n defined by

$$q_n = a_n - b_n e^{-1}. \tag{9.74}$$

Mathematica yields the first few values

$$\begin{aligned} a_1 &= 1, & b_1 &= 1, \\ a_2 &= 3, & b_2 &= 4, \\ a_3 &= 11, & b_3 &= 17, \\ a_4 &= 50, & b_4 &= 84, \\ a_5 &= 274, & b_4 &= 485. \end{aligned}$$

In particular, develop recurrences, explore divisibility properties, examine their growth, and so on.

10. Study the integral

$$I_n = \int_0^1 \frac{(1-x)^n\,dx}{(1+x^2)\log x}. \tag{9.75}$$

Use a symbolic language to check that

$$I_n = \log a_n + b_n \log \pi + c_n \log \Gamma(\tfrac{1}{4}) + d_n \log \Gamma(\tfrac{3}{4}), \tag{9.76}$$

for $a_n \in \mathbb{Q}$ and integers b_n, c_n, d_n. Observe that $c_n = -d_n$ and that $c_{4n+2} = d_{4n+2} = 0$. Explain this.

11. Changes of variables are a powerful tool for the evaluation of definite integral. Sometimes they produce unexpected results. One of them is illustrated in this exercise.

(a) Let R be a rational function with real coefficients. Assume that the integral

$$I = \int_{-\infty}^{\infty} R(x)\,dx \tag{9.77}$$

is convergent. Introduce the change of variables

$$y = \frac{x^2-1}{2x} \tag{9.78}$$

to obtain

$$I = \int_{-\infty}^{\infty} R_1(y)dy, \tag{9.79}$$

where

$$R_1(y) = R(y-\sqrt{y^2-1})\left(1-\frac{y}{\sqrt{y^2+1}}\right) + R(y+\sqrt{y^2-1})\left(1+\frac{y}{\sqrt{y^2+1}}\right). \tag{9.80}$$

Check that R_1 is again a rational function. The degree of R_1 is at most the degree of R.

(b) Discuss the result of part (a) in the special case

$$R(x) = \frac{1}{ax^2+bx+c}. \tag{9.81}$$

The convergence of the integral requires that the *discriminant*

$$D(a,b,c) := b^2 - 4ac \tag{9.82}$$

be negative. Conclude that

$$\int_{-\infty}^{\infty} \frac{dx}{ax^2+bx+c} = \int_{-\infty}^{\infty} \frac{dx}{a_1x^2+b_1x+c_1}, \tag{9.83}$$

where

$$\begin{aligned} a_1 &= \frac{2ac}{a+c}, \\ b_1 &= -\frac{b(a-c)}{a+c}, \\ c_1 &= \frac{(a+c)^2-b^2}{a+c}. \end{aligned} \tag{9.84}$$

This is the rational version of the classical *elliptic Landen transformation*: The elliptic integral

$$G(a,b) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{a^2\cos^2\theta + b^2\sin^2\theta}} \tag{9.85}$$

is invariant under the transformation

$$a_1 = \frac{a+b}{2} \text{ and } b_1 = \sqrt{ab}. \tag{9.86}$$

(c) Check that the discriminant D is preserved by (9.84), that is, $D(a_1,b_1,c_1) = D(a,b,c)$.

(d) Iterate (9.84) to produce a sequence (a_n, b_n, c_n) such that the quadratic integral is preserved. Prove, or convince yourself, that there exists a number L such that

$$a_n \to L, \quad L, \quad b_n \to 0, \quad c_n \to L. \tag{9.87}$$

Use the invariance of the integral to conclude that

$$I = \frac{\pi}{L}. \tag{9.88}$$

This allows you to evaluate the integral I by computing the iterates of (9.84).

(e) Use a symbolic language to develop transformations for the integral

$$U_6 := \int_0^\infty \frac{cx^4+dx^2+e}{x^6+ax^4+bx^2+1}. \tag{9.89}$$

The denominator of the integrand has been normalized to be monic and have constant term 1. This was the original integral discussed in [43]. The iteration of this transformation appears in [87].

The classical elliptic Landen transformation is at the center of the arithmetic geometric mean (AGM). Many good things have come from here. We expect the same to happen with these rational versions.

The rational Landen transformations were developed originally in [43], and the details of the example discussed in this exercise appear in [206, 207]. The reader will find in [52] and [211] general information about the AGM.

12. (Some unresolved integrals.) A *box integral* [19] is an expectation

$$\langle|\vec{r}-\vec{q}|^s\rangle = \int_0^1 \cdots \int_0^1 \left((r_1-q_1)^2+\cdots+(r_n-q_n)^2\right)^{s/2} dr_1\cdots dr_n,$$

where $\vec{r}$ runs over the unit n-cube, with $\vec{q}$ and s fixed, such as the following expectations of distance-from-vertex (i.e., $\vec{q}=0, s=1$) in dimensions one through four:

$$\begin{aligned}
B_1 &= \frac{1}{2},\\
B_2 &= \frac{\sqrt{2}}{3}+\frac{1}{3}\log\left(\sqrt{2}+1\right),\\
B_3 &= \frac{\sqrt{3}}{4}+\frac{1}{2}\log\left(2+\sqrt{3}\right)-\frac{\pi}{24},\\
B_4 &= \frac{2}{5}+\frac{7}{20}\pi\sqrt{2}-\frac{1}{20}\pi\log\left(1+\sqrt{2}\right)\\
&\quad +\log(3)-\frac{7}{5}\sqrt{2}\arctan\left(\sqrt{2}\right)+\frac{1}{10}\mathcal{K}_0,
\end{aligned}$$

where $\mathcal{K}_0$ is given by

$$\begin{aligned}
\mathcal{K}_0 &:= \int_0^1 \frac{\log(1+\sqrt{3+y^2})-\log(-1+\sqrt{3+y^2})}{1+y^2}\,dy\\
&= 2\int_0^1 \frac{\operatorname{arctanh}\left(\frac{1}{\sqrt{3+y^2}}\right)}{1+y^2}\,dy.
\end{aligned}$$

Three other unresolved integrals $\mathcal{K}_1, \mathcal{K}_2$, and $\mathcal{K}_3$ from [19] are

$$\mathcal{K}_1 := \int_3^4 \frac{\operatorname{arcsec}(x)}{\sqrt{x^2-4x+3}}\,dx,$$

$$\begin{aligned}
\mathcal{K}_2 &:= \int_0^{\pi/4}\sqrt{1+\sec^2(a)}\,\arctan\left(\frac{1}{\sqrt{1+\sec^2(a)}}\right)da\\
&= \frac{\pi^2}{16}-\sum_{m=1}^{\infty}\frac{(-1)^m}{2^m}\sum_{k=1}^{m-1}\frac{\binom{-(m-k)}{k}}{2(m-k)+1}\sum_{j=0}^{k-1}\frac{(-1)^j}{2j+1},
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{K}_3 &:= \int_0^{\pi/4}\int_0^{\pi/4}\sqrt{1+\sec^2(a)+\sec^2(b)}\,da\,db\\
&= -\sqrt{3}\sum_{n=0}^{\infty}\frac{\binom{2n}{n}/(2n-1)}{12^n}\sum_{k=0}^{n}\binom{n}{k}\\
&\quad\times\left(\frac{\pi}{4}-\sum_{j=0}^{k-1}\frac{(-1)^j}{2j+1}\right)\left(\frac{\pi}{4}-\sum_{j=0}^{n-k-1}\frac{(-1)^j}{2j+1}.\right).
\end{aligned}$$

(a) Verify the values given for B_1, B_2, B_3, and B_4. For B_4 this requires a good integration method for box integrals, see [19].

(b) Can one find closed-forms for all or any of these integrals?

Exercises for Chapter 8

1. (Computing values of $\mathscr{W}(a,b,c)$.)

   (a) For $r+s+t=6$ the only terms we need to consider are $\zeta(6)$ and $\zeta^2(3)$, since $\zeta(6), \zeta(4), \zeta(2)$, and $\zeta^3(2)$ are all rational multiples of π^6. We recovered

   $$\mathscr{W}(3,2,1) = \int_0^1 \frac{\mathrm{Li}_3(x)\,\mathrm{Li}_2(x)}{x}\,dx = \frac{1}{2}\zeta^2(3),$$

   consistent with the equation below (8.22). Find all weight-six and weight-seven evaluations.

   (b) At weight eight, one irreducible must be introduced, say $\zeta(6,2)$.

2. Prove the inequalities given in the preparatory Lemma 8.6 used for Hilbert's inequality of Theorem 8.7.

3. Show, as outlined in the text, that the constant in Hardy's inequality given in Theorem 8.11 is best possible.

4. Show that $\sigma_n := \frac{2}{\pi}\int_0^\infty \mathrm{sinc}^n$ is strictly decreasing. Aliev [4] uses this among other tools to show that, for any nonzero a in Z^n, there exist linearly independent vectors (x_k) in Z^n with $\langle a, x_k\rangle = 0$ such that

   $$\|x_1\|\|x_2\|\cdots\|x_n\| < \frac{\|a\|}{\sigma_n}.$$

5. Ramanujan's AGM continued fraction is the object

   $$\mathscr{R}_\eta(a,b) = \cfrac{a}{\eta + \cfrac{b^2}{\eta + \cfrac{4a^2}{\eta + \cfrac{9b^2}{\eta + \ddots}}}},$$

   certainly valid for $a,b,\eta > 0$.

   Our discussion of $\mathscr{R}_\eta$ follows [65, 66, 51]. It enjoys attractive algebraic properties such as a striking arithmetic-geometric mean relation

   $$\mathscr{R}_\eta\left(\frac{a+b}{2}, \sqrt{ab}\right) = \frac{\mathscr{R}_\eta(a,b) + \mathscr{R}_\eta(b,a)}{2} \tag{9.90}$$

   and has elegant links with elliptic-function theory [51]. We may restrict attention to $\eta = 1$, since $\mathscr{R}_\eta(a,b) = \mathscr{R}_1(a/\eta, b/\eta)$. Now $\mathscr{R}_1$ is far from easy to compute naively.

(a) Indeed, inspection of $\mathscr{R}_1$ yields the *reduced continued fraction* form:

$$\mathscr{R}_1(a,b) = \frac{a}{[c_0; c_1, c_2, c_3, \ldots]}$$
$$:= \cfrac{c}{c_0 + \cfrac{1}{c_1 + \cfrac{1}{c_2 + \cfrac{1}{c_3 + \ddots}}}}$$

where the c_i are all positive real numbers.

(b) Show that c_n satisfies

$$c_n = \frac{n!^2}{(n/2)!^4}\, 4^{-n}\, \frac{b^n}{a^n} \quad \sim \quad \frac{2}{\pi \mathbf{n}}\, \frac{b^n}{a^n}$$

for even n, while for odd n

$$c_n = \frac{((n-1)/2!)^4}{n!^2}\, 4^{n-1}\, \frac{a^{n-1}}{b^{n+1}} \quad \sim \quad \frac{\pi}{2\, ab\, \mathbf{n}}\, \frac{a^n}{b^n}.$$

This representation leads immediately to a proof that, for any positive real pair a, b, the fraction $\mathscr{R}_1(a,b)$ converges. Indeed, by the *Seidel-Stern theorem* [65, 66], a reduced continued fraction converges if and only if $\sum c_i$ diverges. In our case, such divergence is evident for every choice of real $a, b > 0$. Note that for $a = b$ divergence of $\sum c_i$ is only *logarithmic*; hence, and somewhat surprisingly, this is the hardest case to compute.

(c) There are, however, beautiful numerical series involving the *complete elliptic integral*

$$K(k) = \int_0^{\pi/2} \frac{1}{\sqrt{1 - k^2 \sin^2\theta}}\, d\theta.$$

Below we write $\mathrm{K} := \mathrm{K}(k)$ and $\mathrm{K}' := \mathrm{K}(k')$ with $k' := \sqrt{1-k^2}$.

For $0 < b < a$ and $k := b/a$, we have

$$\mathscr{R}_1(a,b) = \frac{\pi a \mathrm{K}}{2} \sum_{n \in Z} \frac{\operatorname{sech}\left(n\pi \frac{\mathrm{K}'}{\mathrm{K}}\right)}{\mathrm{K}^2 + \pi^2 a^2 n^2}. \tag{9.91}$$

Correspondingly, for $0 < a < b$ and $k := a/b$, we have

$$\mathscr{R}_1(a,b) = 2\pi b \mathrm{K} \sum_{n \in Z, \mathrm{odd}} \frac{\operatorname{sech}\left(n\pi \frac{\mathrm{K}'}{2\mathrm{K}}\right)}{4\mathrm{K}^2 + \pi^2 b^2 n^2}. \tag{9.92}$$

Since K is fast computable—and well implemented in *Maple* and *Mathematica*—for a and b not too close these formulas are very effective. Moreover, Poisson transformation, for $0 < b < a$, yields

$$\mathscr{R}_1(a,b) = \mathscr{R}_1\left(\frac{\pi a}{2\mathrm{K}'}, \frac{\pi a}{2\mathrm{K}'}\right) + \frac{\pi}{\cos\frac{\mathrm{K}'}{a}}\,\frac{1}{e^{2\mathrm{K}/a}-1}$$
$$+\,8\pi a \mathrm{K}' \sum_{0<d\in Z,\mathrm{odd}} \frac{(-1)^{(d-1)/2}}{4\mathrm{K}'^2 - \pi^2 d^2 a^2}\,\frac{1}{e^{\pi d \mathrm{K}/\mathrm{K}'}-1}.$$

Thus, once we obtain an effective formula for $\mathscr{R}(a) := \mathscr{R}_1(a,a)$, we can compute $\mathscr{R}_1$ for all $a,b > 0$ since Ramanujan's identity (9.90) allows us to compute only with $a > b > 0$.

This is the gist of the next exercise.

6. (Closed forms for $\mathscr{R}$.) By viewing (9.91) as a Riemann sum as $b \to a^-$, prove that for all $a > 0$
$$\mathscr{R}(a) = \int_0^\infty \frac{\operatorname{sech}\left(\frac{\pi x}{2a}\right)}{1+x^2}\,dx.$$
   (a) Derive that
$$\begin{aligned}
\mathscr{R}(a) &= 2a\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{1+(2k-1)a} \\
&= \frac{1}{2}\left(\psi\left(\frac{3}{4}+\frac{1}{4a}\right) - \psi\left(\frac{1}{4}+\frac{1}{4a}\right)\right) \\
&= \frac{2a}{1+a}\,{}_2\mathrm{F}_1\left(\frac{1}{2a}+\frac{1}{2}, 1; \frac{1}{2a}+\frac{3}{2}; -1\right) \\
&= 2\int_0^1 \frac{t^{1/a}}{1+t^2}\,dt.
\end{aligned}$$
   (b) Conclude that
$$\mathscr{R}(a) = \int_0^\infty e^{-x/a}\operatorname{sech}(x)\,dx.$$
   (c) Show that
$$\mathscr{R}(a) = \frac{2a}{1+a} - \mathscr{R}\left(\frac{a}{1+2a}\right).$$
   (d) Determine the value of $\mathscr{R}(n)$ for $n = 1,2,3,\ldots$ or even for n rational. For example, $\mathscr{R}(1) = \log 2$, $\mathscr{R}(3) = \pi/\sqrt{3} - \log 2$, and $\mathscr{R}(3/2) = \pi + \sqrt{3}\log(2-\sqrt{3})$. No closed form is known for $\mathscr{R}_\infty(a,b)$ when $a \neq b$.

7. The values of $\zeta(2,1), \zeta(2,-1), \zeta(-2,1)$, and $\zeta(-2,-1)$ all reduce to sums of products of one-dimensional (alternating) zeta functions. Thus, the only possible basis elements are $\zeta(3)$ and $\zeta(2)\log(2)$. Hence, recover
$$\zeta(2,1) = \zeta(3), \quad \zeta(-2,1) = \frac{1}{8}\zeta(3),$$

$$\zeta(2,-1) = \zeta(3) - \frac{3}{2}\zeta(2)\log(2),$$
$$\zeta(-2,-1) = \frac{3}{2}\zeta(2)\log(2) - \frac{13}{8}\zeta(3). \tag{9.93}$$

8. (Uses of the Dilogarithm and Trilogarithm.) We describe material taken from [57].

   (a) Consider the power series

   $$J(x) := \zeta(2,1;x) = \sum_{n>k>0} \frac{x^n}{n^2 k}, \qquad 0 \le x \le 1,$$

   and show that

   $$J(x) = \int_0^x \frac{dt}{t} \int_0^t \frac{du}{1-u} \int_0^v \frac{dv}{1-v} = \int_0^x \frac{\log^2(1-t)}{2t}\,dt.$$

   (b) *Maple* readily evaluates

   $$\int_0^x \frac{\log^2(1-t)}{2t}\,dt = \zeta(3) + \frac{1}{2}\log^2(1-x)\log(x) + \log(1-x)\mathrm{Li}_2(1-x) - \mathrm{Li}_3(1-x), \tag{9.94}$$

   where $\mathrm{Li}_s(x) = \sum_{n=1}^{\infty} x^n/n^s$ is the classical polylogarithm, as before.

   (c) Verify (9.94) by differentiating both sides by hand and checking that (9.94) holds as $x \to 0+$. Thus, deduce

   $$J(x) = \zeta(3) + \frac{1}{2}\log^2(1-x)\log(x) + \log(1-x)\mathrm{Li}_2(1-x) - \mathrm{Li}_3(1-x).$$

   Let $x \to 1-$ to prove (9.93).

   (d) In *Ramanujan's Notebooks*, we also find that

   $$J(-z) + J(-1/z) = -\frac{1}{6}\log^3 z - \mathrm{Li}_2(-z)\log z + \mathrm{Li}_3(-z) + \zeta(3), \tag{9.95}$$

   and

   $$J(1-z) = \frac{1}{2}\log^2 z\log(z-1) - \frac{1}{3}\log^3 z - \mathrm{Li}_2(1/z)\log z - \mathrm{Li}_3(1/z) + \zeta(3). \tag{9.96}$$

   (e) Put $z = 1$ in (9.95) and employ the well-known *dilogarithm evaluation*

   $$\mathrm{Li}_2(-1) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} = -\frac{\pi^2}{12}$$

   to obtain (9.10).

(f) Put $z = 2$ in (9.96) and employ Euler's *dilogarithm evaluation*

$$\mathrm{Li}_2\left(\frac{1}{2}\right) = \sum_{n=1}^{\infty} \frac{1}{n^2\, 2^n} = \frac{\pi^2}{12} - \frac{1}{2}\log^2 2$$

along with Landen's *trilogarithm evaluation* (see Lewin [198] or [199])

$$\mathrm{Li}_3\left(\frac{1}{2}\right) = \sum_{n=1}^{\infty} \frac{1}{n^3\, 2^n} = \frac{7}{8}\zeta(3) - \frac{\pi^2}{12}\log 2 + \frac{1}{6}\log^3 2$$

to obtain (9.10) yet again.

(g) These evaluations follow respectively from the functional equations

$$\mathrm{Li}_2(x) + \mathrm{Li}_2(1-x) \quad = \quad \zeta(2) + \log(x)\log(1-x) \tag{9.97}$$

and

$$\mathrm{Li}_3(x) + \mathrm{Li}_3(1-x) + \mathrm{Li}_3(x/(x-1)) = \tag{9.98}$$
$$\zeta(3) - \frac{1}{2}\log(x)\log^2(1-x) + \zeta(2)\log(1-x) + \frac{1}{6}\log^3(1-x).$$

Prove both of these by symbolically determining that they have equal derivatives on both sides.

(h) Once the component functions in (9.97), (9.98), or (9.13) are known, the coefficients can be deduced by computing each term to high precision with a common transcendental value of x and employing a linear relations finding algorithm. This is also an excellent way to error-correct.

9. (AMM Problem 11115, November 2004.) Evaluate the limit of

$$E_m := \left(\sum_{k=1}^{m} \frac{1}{k}\right)^2 - \sum_{k=1}^{m} \frac{\sum_{j=1}^{\max(k,m-k)} 1/j}{k},$$

as m goes to ∞.

(a) First, show the limit exists.

Hint: Exhibit E_m as a double Riemann sum for the integral following:

$$E_m = \frac{1}{m}\sum_{k=1}^{m} \frac{\frac{1}{m}\sum_{1+\max(k,m-k)}^{m} \frac{1}{j/m}}{k/m},$$

which converges to

$$\int_0^1 \frac{1}{x}\int_{(1-x)\vee x}^{1} \frac{1}{y}\,dy\,dx = -\int_0^{1/2} \frac{\log(1-x)}{(1-x)}\frac{dx}{x}$$
$$= 0.8224670336\ldots.$$

We note that the `identify` function in *Maple* will identify the constant from the numeric value of the integral: 0.8224670336.... This is much more difficult from the original sum where 10,000 terms only provides 0.82236685....

(b)

$$-\int_0^{1/2} \frac{\log(1-x)}{(1-x)} \frac{dx}{x} = \frac{\pi^2}{12},$$

as is known to both *Maple* and *Mathematica* and can be obtained from the value of dilogarithm at $1/2$, or by other methods. Indeed, with the assumption that $0 < t < 1$, *Maple* returns

$$-\int_0^{t} \frac{\log(1-x)}{(1-x)} \frac{dx}{x} = \frac{1}{2}\log^2(1-t) + \mathrm{dilog}(1-t),$$

as differentiation yet again confirms. (Note that *Maple* uses $\mathrm{dilog}(x) = \mathrm{Li}_2(1-x)$.) Now use (f) of the previous exercise.

(c) Evaluate

$$\sum_{n=1}^{\infty} \frac{H_n}{n\,2^n} \text{ and } \sum_{n=1}^{\infty} \frac{H_{n-1}}{n\,2^n},$$

with $H_n := 1 + 1/2 + \cdots 1/n$.

10. (Some Ising integrals.) Define

$$I_n := \int_0^{\infty} \frac{\left(\prod_{n\geq k>j\geq 1} \frac{u_k-u_j}{u_k+u_j}\right)^2}{\left(\sum_{j=1}^{n} u_j + 1/u_j\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}.$$

(a) Use the symmetry of the I_n integrands to reduce to the simplex where $u_k > u_{k+1}$, and then use the change of variables $u_k := \prod_{i=1}^{k} t_i$ to represent the integral as

$$I_n = 2\int_0^1 \iota_n \, dt_2\, dt_3 \cdots dt_n$$

with

$$\iota_n(t_2, t_3 \ldots, t_n) := n! \left(\prod_{n\geq k>j\geq 1} \frac{u_k/u_j - 1}{u_k/u_j + 1} \right)^2 \times \frac{1}{(1+\sum_{k=2}^{n} w_k)(1+\sum_{k=2}^{n} v_k)},$$

where

$$w_k := \prod_{i=2}^{k} t_i, \quad v_k := \prod_{i=k}^{n} t_i,$$

since the integral in $t_1 = u_1$ is now easy to obtain.

(b) Determine that $\iota_1 = 1$ and $\iota_2 = 2!\,(t_2-1)^2/(t_2+1)^4$ while

$$\iota_3 = 3!\, \frac{(t_2-1)^2 (t_2t_3-1)^2 (t_3-1)^2}{(t_2+1)^2 (t_2t_3+1)^2 (t_3+1)^2 (t_2+t_2t_3+1)(t_2t_3+t_3+1)}.$$

(c) Hence,

$$I_2 = 4\int_0^1 \frac{(x-1)^2}{(x+1)^4}\,dx = \frac{1}{6},$$

$$I_3 = 24\int_0^1\int_0^x \iota_3(x,y)\,dx\,dy,$$

which *Maple* can reduce to

$$1+\zeta(2)-\frac{27}{8}L_{-3}(2)$$

(most easily from the same integral over the positive orthant, which is six times the integral on the square). The code

```
p:=(x-1)^2*(x-y)^2*(y-1)^2/(x+1)^2/(x+y)^2/(y+1)^2
                                  /(1+y+x)/(y+x+x*y):
Int(Int(p, x = 0 .. infinity),y = 0 .. infinity):
evalc(value(%));
```

returns

$$18\,i\,\mathrm{dilog}\left(1/2-1/2\,i\sqrt{3}\right)\sqrt{3}-18\,i\,\mathrm{dilog}\left(1/2+1/2\,i\sqrt{3}\right)\sqrt{3}$$
$$+24+4\pi^2.$$

The value of I_4 is known to be $-1/6+4\pi^2/9+7/2\,\zeta(3)$ but the status of higher values is open [265].

11. (Levy Constants.) [136] Let p_n/q_n be the nth convergent of a number $\alpha>0$. Levy showed in 1929 that $\lambda(\alpha) := \lim_{n\to\infty}\frac{\log q_n}{n}$ exists and is a constant, $\overline{\lambda}$, for almost all irrationals. It is also known that $\lambda(\beta)$ exists for all quadratic irrationals β and is dense in $[\log G,\infty]$ where G is the golden mean [285].

(a) Numerically explore the constant and attempt to identify $\overline{\lambda}$ numerically and then symbolically.

(b) Explore whether either π or e appears to behave "normally."

(c) For a quadratic β with purely-periodic part fraction $[b_1,b_2,\ldots b_N]$, show that

$$\lambda(\beta) = \frac{\log\sigma(B_N)}{N},$$

where σ denotes the spectral radius and B_N is the matrix

$$\prod_{k=1}^{N}\begin{bmatrix} b_k & 1\\ 1 & 0\end{bmatrix}.$$

Hint: $\overline{\lambda}\approx 1.1865691104156$.

Additional Exercises

Here we collect various additional examples and exercises.

1. (Szegő curves.) While the exponential has no zeroes, its partial Taylor series at zero do. We wish to explore the zeroes of such partial sums of the exponential: $\{s_n(z)\}$ where $s_n(z) := \sum_{k=0}^{n} z^k/k!$.

   (a) Begin by computing and plotting the zeroes of s_n for various values of n as in Figure 9.2. Remarkably, the shape of the curves appears very stable and regular. Indeed, doing the same for the normalized curves as in Figure 9.3 strongly suggests there is a limit curve.

   Maple code to draw such zeroes is simple:

```
draw:=(l,N)->complexplot([fsolve(l(N),x,complex)],
                              style=point,color=black):
sn:=N->sum((N*x)^n/n!,n=1..N):draw(sn(50));
```

   (b) In 1924, Szegő showed (with no such tools) that the zeroes of the *normalized partial sums*, $s_n(nz)$, of e^z tended to the curve, now called the *Szegő curve* S, shown in Figure 9.4, where

$$S := \left\{ z \in \mathbf{C} : |ze^{1-z}| = 1 \text{ and } |z| \leq 1 \right\}.$$

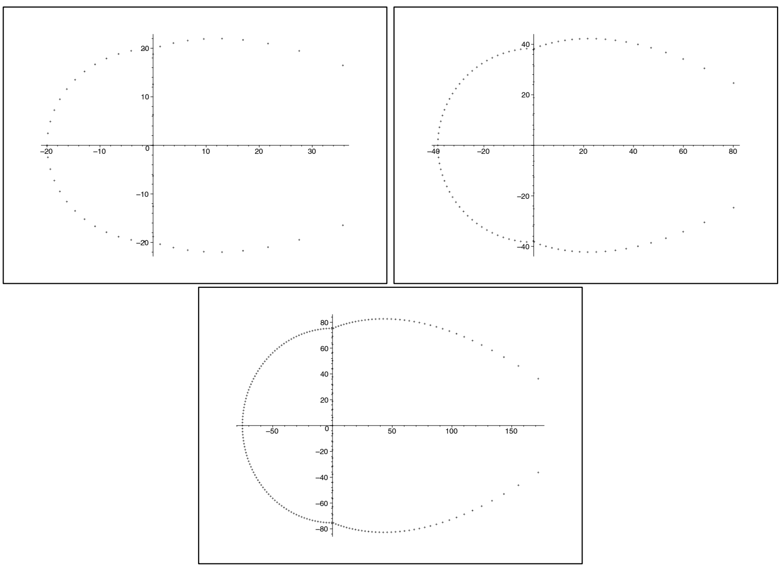


Figure 9.2. The zeroes of s_n for $n = 50, 100, 200$.

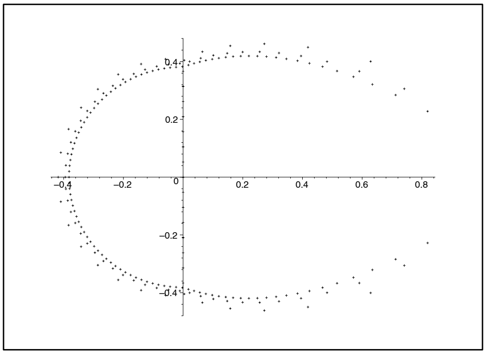


Figure 9.3. The zeroes of the normalized s_n for $n = 30, 60, 120$.

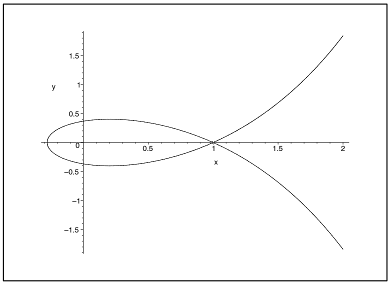


Figure 9.4. The Szegő curve for $\exp(z)$.

Via modern weighted potential theory, Pritzger and Varga [240] recover these zero distribution results of Szegő, along with an asymptotic formula for the weighted partial sums $\{e^{-nz}s_n(nz)\}_{n=0}^{\infty}$.

They go on to show that $G := \operatorname{Int} S$ is the largest universal domain such that the weighted polynomials $e^{-nz}P_n(z)$ are dense in the set of functions analytic in G. More generally, they show that if $f(z)$ is analytic in G and continuous on $\overline{G}$ with $f(1) = 0$, then there is a sequence of polynomials $\{P_n(z)\}_{n=0}^{\infty}$, with $\deg P_n \leq n$, such that

$$\lim_{n\to\infty} \|e^{-nz}P_n(z) - f(z)\|_{\overline{G}} = 0,$$

where $\|\cdot\|_{\overline{G}}$ denotes the supremum norm on $\overline{G}$. The reader may wish to follow up by consulting Zemyan‘s recent article [289].

(c) Explore what happens for other normalized Taylor polynomials.

2. (Clausen's function and the figure-eight knot complement volume.) As discussed in [50], the volume of the figure-eight knot complement, which we take to be defined by the *log sine integral*

$$V = -2\int_0^{\pi/3} \log\left(2\sin\left(\frac{t}{2}\right)\right) dt, \tag{9.99}$$

is also given by the ternary BBP formula

$$\frac{3\sqrt{3}}{2}V = \sum_{k=0}^{\infty}\left(\frac{-1}{27}\right)^k \left(\frac{9}{(6k+1)^2} - \frac{9}{(6k+2)^2} - \frac{12}{(6k+3)^2} - \frac{3}{(6k+4)^2} + \frac{1}{(6k+5)^2}\right). \tag{9.100}$$

Recall that the *Clausen function* is

$$\mathrm{Cl}_2(\theta) = \sum_{n>0} \frac{\sin(n\theta)}{n^2}, \tag{9.101}$$

which satisfies $\mathrm{Cl}_2(\pi/2) = G$. Requisite details about Clausen's function are to be found in Lewin [199].

(a) Show that integration of (9.99) gives

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

(b) Show that a hypergeometric equivalent formulation of (9.100) is

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

With some effort this is expressible in dilogarithms leading to

$$\begin{aligned} V \stackrel{?}{=} \mathrm{Im}\left\{4\,\mathrm{Li}_2\left(\frac{i\sqrt{3}}{3}\right) - \frac{8}{3}\mathrm{Li}_2\left(\frac{i\sqrt{3}}{9}\right) \right. \\ \left. +\mathrm{Li}_2\left(\frac{1}{2} - \frac{i\sqrt{3}}{6}\right) + 8\,\mathrm{Li}_2\left(-\frac{1}{2} + \frac{i\sqrt{3}}{6}\right)\right\}. \end{aligned}$$

(c) Now, Lewin in Equation (5.5) of [199] gives

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

where $\omega = \arctan(r \sin\theta/(1 - r\cos\theta))$. Using this, a proof that (9.100) holds is reduced to showing that, with $\alpha = \arctan(\sqrt{3}/9)$,

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

which is true by applying the two variable identities for Clausen's function given in Equations (4.61) and (4.63) of [199], with $\theta = \pi/3$.

3. (The origin of formula (1.1).) A much harder unproven identity is

$$\frac{7\sqrt{7}}{4} L_{-7}(2) = 3\,\mathrm{Cl}_2(\alpha) - 3\,\mathrm{Cl}_2(2\,\alpha) + \mathrm{Cl}_2(3\,\alpha) \tag{9.102}$$

with $\alpha = 2\arctan\left(\sqrt{7}\right)$. Show that (9.102) is equivalent to (1.1); indeed, it is the form in which the identity was originally found using PSLQ.

4. Recall that

$$\sum_{n=1}^{\infty} \frac{1}{2^n n^2} = \mathrm{Li}_2\left(\frac{1}{2}\right) = \frac{1}{2}\zeta(2) - \frac{1}{12}\log^2(2),$$

and verify, as discovered by Sergey Zlobin using PSLQ in *EZface*, that

$$\sum_{n=1}^{\infty} \frac{1}{2^n n^2} \sum_{m=1}^{n-1} \frac{1}{m^2} = \frac{1}{24}\log^4(2) - \frac{1}{4}\zeta(2)\log^2(2) + \frac{1}{4}\zeta(3)\log(2) + \frac{1}{16}\zeta(4).$$

Find a corresponding formula for $\sum_{n=1}^{\infty} \frac{1}{2^n n^2} \sum_{m=1}^{n-1} \frac{1}{m^2} \sum_{p=1}^{m-1} \frac{1}{p^2}$.

Hint: Compute the coefficient of z^{2n} in $(A(z) + A(-z))/2$, where

$$A(z) := \frac{\Gamma(1/2)}{\Gamma(1 + z/2)\Gamma(1/2 - z/2)} = \frac{2}{B(1 + z/2, 1/2 - z/2)}.$$

5. (An extremal problem.) For $t > 0$, $a > 1$, let

$$f_a(t) := a^{-t} + a^{-1/t},$$

and set $f_a(0) := 1$ (the limiting value). Show that

$$\sup_{t \geq 1} f_a(t) = \max\left(\frac{2}{a}, 1\right).$$

Hint: Since $f_a(t) = f_a(1/t)$, and $f_a(t)$ is continuous on $[0, \infty)$ and differentiable on $(0, \infty)$, it suffices to show that $f_a(t)$ has a unique critical point (necessarily a minimum) in $(0, 1)$. (See Figure 9.5.) In that case $f_a(t)$ must assume its maximum value at the larger of $f_a(0) = 1$ and $f_a(1) = 2/a$. Now the condition for a critical point becomes $a^{(t^2-1)/2t} = t$, and taking logs this is

$$(t^2 - 1)\log(a) = 2t\log(t).$$

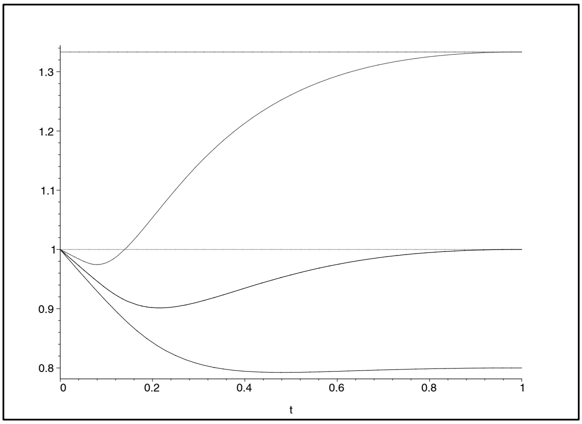


Figure 9.5. The function f_a on $[0,1]$ for $1 < a < 2$, $a = 2$, and $a > 2$.

Substituting $t = \sqrt{u}$, we see that it suffices to show that there is a unique $u \in (0,1)$ satisfying

$$g_a(u) := (u-1)\log(a) = \sqrt{u}\log(u) =: h(u).$$

Since $g_a(u)$ is affine, while $h(u)$ is convex on $[0,1]$, and $-\log(a) = g_a(0) < h(0) = 0 = h(1) = g_a(1)$, it follows that there is a *unique* $u \in (0,1)$ such that $g_a(u) = h(u)$, as illustrated in Figure 9.6.

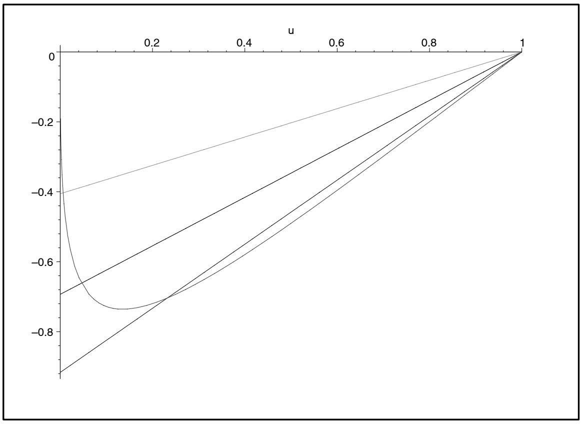


Figure 9.6. The functions h and g_a on $[0,1]$ for $1 < a < 2$, $a = 2$, and $a > 2$.

6. (Centrally symmetric polytopes [31, p. 276].) No example is known of a d-dimensional centrally symmetric polytope with fewer than 3^d faces. Can one exist? The square and cube have 9 and 27 faces, respectively.
7. (Minkowski's convex body theorem [31, p. 295].) One of the most beautiful and potent results relating geometry and number theory is Minkowski's theorem, which

asserts that in $\mathbb{R}^d$ a (compact) convex body A must meet an integer lattice Λ as soon as $\operatorname{vol} A > 2^d \det \Lambda$. (That $\operatorname{vol} A \geq 2^d \det \Lambda$ suffices in the compact case.)

(a) Establish Siegel's result that

$$2^d = \operatorname{vol} A + \frac{4^d}{\operatorname{vol} A} \sum_{u \in \mathbb{Z}^d} \left| \int_{A/2} \exp\{-2\pi i \langle u, x \rangle\} \right|^2 .$$

Hint: Again Fourier techniques are suggested. Use Parseval's formula applied to the function

$$\sum_{u \in \mathbb{Z}^d} \chi_{u+A/2}.$$

(b) Deduce Minkowski's theorem.

(c) Show this fails for nonsymmetric bodies and that it is best possible (in two dimensions).

8. (Inequalities for sinc integrals.) Suppose that $\{a_n\}$ is a sequence of positive numbers. Let $s_n := \sum_{k=1}^n a_k$, and set

$$\tau_n := \int_0^\infty \prod_{k=0}^n \operatorname{sinc}(a_k x)\, dx.$$

Show that

(a)
$$0 < \tau_n \leq \frac{\pi}{2\, a_0},$$
with equality if $n = 0$, or if $a_0 \geq s_n$ when $n \geq 1$.

(b) If $a_{n+1} \leq a_0 < s_n$ with $n \geq 1$, then

$$0 < \tau_{n+1} \leq \tau_n < \frac{1}{a_0} \frac{\pi}{2}.$$

(c) If $a_0 < s_{n_0}$ with $n_0 \geq 1$ and $\sum_{k=0}^\infty a_k^2 < \infty$, then there is an integer $n_1 \geq n_0$ such that

$$\tau_n \geq \int_0^\infty \prod_{k=0}^\infty \operatorname{sinc}(a_k x)\, dx \geq \int_0^\infty \prod_{k=0}^\infty \operatorname{sinc}^2(a_k x)\, dx > 0$$

for all $n \geq n_1$.

Observe that applying the result to different permutations of the parameters will in general yield different inequalities.

Proof:

(a) We know that $\tau_0 = \pi/(2a_0)$ is a standard result (proven, e.g., by contour integration or Fourier analysis with the integral in question being improper). Assume therefore that $n \geq 1$, and define the following convolutions

$$F_0 := \frac{1}{a_0}\sqrt{\frac{\pi}{2}}\chi_{a_0}, \quad F_n := (\sqrt{2\pi})^{1-n} f_1 * f_2 * \cdots * f_n,$$

where $f_n := \frac{1}{a_n}\sqrt{\frac{\pi}{2}}\chi_{a_n}$.

By induction, for $n \geq 1, F_n(x)$ is even, vanishes on $(-\infty, -s_n) \cup (s_n, \infty)$, and is positive on $(-s_n, s_n)$. Moreover, $F_{n+1} = \frac{1}{\sqrt{2\pi}} F_n * f_{n+1}$, so that

$$\begin{aligned} F_{n+1}(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F_n(x-t) f_{n+1}(t)\, dt \\ &= \frac{1}{2a_{n+1}} \int_{x-a_{n+1}}^{x+a_{n+1}} F_n(u)\, du. \end{aligned}$$

Hence, $F_{n+1}(x)$ is absolutely continuous on $(-\infty, \infty)$ and, for almost all $x \in (-\infty, \infty)$,

$$\begin{aligned} 2a_{n+1}F'_{n+1}(x) &= F_n(x+a_{n+1}) - F_n(x-a_{n+1}) \\ &= F_n(x+a_{n+1}) - F_n(a_{n+1}-x). \end{aligned}$$

Since $(x+a_{n+1}) \geq \max\{(x-a_{n+1}), (a_{n+1}-x)\} \geq 0$ when $x > 0$, it follows that if $F_n(x)$ is monotone nonincreasing on $(0, \infty)$, then $F'_{n+1}(x) \leq 0$ for almost all $x \in (0, \infty)$, and so $F_{n+1}(x)$ is monotone nonincreasing on $(0, \infty)$. This monotonicity property of F_n on $(0, \infty)$ is therefore established by induction for all $n \geq 1$. Also, F_n is the cosine transform (FCT) of $\sigma_n(x) := \prod_{k=1}^{n} \operatorname{sinc}(a_k x)$, and σ_n is the FCT of F_n. Thus, all our functions and transforms are even and are in $L_1(0, \infty) \cap L_2(0, \infty)$.

Hence, by Parseval's theorem,

$$\tau_n = \int_0^{\infty} F_n(x) F_0(x)\, dx = \frac{1}{a_0}\sqrt{\frac{\pi}{2}} \int_0^{\min(s_n, a_0)} F_n(x)\, dx. \tag{9.103}$$

When $a_0 \geq s_n$, the final term is equal to

$$\frac{1}{a_0}\sqrt{\frac{\pi}{2}}\sqrt{\frac{\pi}{2}}\sigma_n(0) = \frac{1}{a_0}\frac{\pi}{2}$$

since $\sigma_n(x)$ is continuous on $(-\infty, \infty)$; when $a_0 < s_n$, the term is positive and less than $\pi/(2a_0)$ since $F_n(x)$ is positive and continuous for $0 < x < s_n$.

(b) Note again that $F_{n+1} = \frac{1}{\sqrt{2\pi}} F_n * f_{n+1}$, and hence, for $y > 0$,

$$\begin{aligned}
\int_0^y F_{n+1}(x)\,dx &= \frac{1}{\sqrt{2\pi}} \int_0^y dx \int_{-\infty}^{\infty} F_n(x-t) f_{n+1}(t)\,dt \\
&= \frac{1}{2a_{n+1}} \int_0^y dx \int_{-a_{n+1}}^{a_{n+1}} F_n(x-t)\,dt \\
&= \frac{1}{2a_{n+1}} \int_{-a_{n+1}}^{a_{n+1}} dt \int_0^y F_n(x-t)\,dx \\
&= \int_0^y F_n(u)\,du + \frac{1}{2a_{n+1}} (I_1 + I_2),
\end{aligned}$$

where

$$\begin{aligned}
I_1 &:= \int_{-a_{n+1}}^{a_{n+1}} dt \int_{-t}^{0} F_n(u)\,du \quad \text{and} \\
I_2 &:= \int_{-a_{n+1}}^{a_{n+1}} dt \int_{y}^{y-t} F_n(u)\,du.
\end{aligned}$$

Now $I_1 = 0$ since $t \mapsto \int_{-t}^{0} F_n(u)\,du$ is odd, and for $y \geq a_{n+1}$

$$\begin{aligned}
I_2 &= \int_0^{a_{n+1}} dt \int_y^{y-t} F_n(u)\,du + \int_{-a_{n+1}}^{0} dt \int_y^{y-t} F_n(u)\,du \\
&= -\int_0^{a_{n+1}} dt \int_{y-t}^{y} F_n(u)\,du + \int_0^{a_{n+1}} dt \int_y^{y+t} F_n(u)\,du \\
&= \int_0^{a_{n+1}} dt \int_{y-t}^{y} \big(F_n(u+t) - F_n(u)\big)\,du \leq 0
\end{aligned}$$

since $F_n(u)$ is nonincreasing for $u \geq y - t \geq y - a_{n+1} \geq 0$. Hence,

$$\int_0^y F_{n+1}(x)\,dx \leq \int_0^y F_n(x)\,dx \text{ when } a_{n+1} \leq y < s_n. \tag{9.104}$$

It follows from (9.103), and (9.104) with $y = a_0$, that $0 < \tau_{n+1} \leq \tau_n$ if $a_{n+1} \leq a_0 < s_n$.

(c) Let $\rho(x) := \lim_{n\to\infty} \sigma_n^2(x) = \prod_{k=1}^{\infty} \operatorname{sinc}^2(a_k x)$ for $x > 0$. The limit exists since $0 \leq \operatorname{sinc}^2(a_k x) < 1$, and there is a set A differing from $(0,\infty)$ by a countable set such that $0 < \operatorname{sinc}^2(a_k x) < 1$ whenever $x \in A$ and $k = 1, 2, \ldots$. Now

$$\operatorname{sinc}(a_k x) = 1 - \delta_k, \text{ where } 0 \leq \frac{\delta_k}{a_k^2} \to \frac{x^2}{3} \text{ as } k \to \infty,$$

so that $\sum_{k=1}^{\infty} \delta_k < \infty$, and hence, by standard theory of infinite products, $\sigma(x) := \lim_{n\to\infty} \sigma_n(x)$ exists and $\sigma^2(x) = \rho(x) > 0$ for $x \in A$. It follows, by part (b), that

$$\tau_n \geq \int_0^{\infty} \sigma_n^2(x)\,dx \geq \int_0^{\infty} \rho(x)\,dx > 0$$

for all $n \geq n_1$, where $n_1 \geq n_0$ is an integer such that $a_{n+1} \leq a_0$ for all $n \geq n_1$. In addition, by dominated convergence,

$$\lim_{n\to\infty} \tau_n = \int_0^\infty \sigma(x)\,dx \geq \int_0^\infty \rho(x)\,dx,$$

and we are done. □

9. (A discrete dynamical system.) One of the advantages of a symbolic computer package is how accessible it makes initial study of discrete dynamical systems. Recall that a map is *chaotic* if (i) it has a dense set of periodic orbits, (ii) exhibits *sensitive dependence* on initial conditions, and (iii) is *topologically transitive*, meaning that orbits mix completely.

   It is well known that "period three implies chaos" for one-dimensional systems. In particular, Sharkovsky's theorem given in [50, p. 79] implies that a continuous self-map φ of the reals with a period-three point will have periodic points of all orders.

   The following example due to Marc Chamberland shows how completely this fails in $\mathbb{R}^2$. Consider the dynamics $z_{n+1} := \varphi(z_n)$ of the map

$$(u,v) = (y, x^2 - y^2).$$

   Show that

   (a) all points in the open unit square are attracted to zero;

   (b) there is a 3-cycle but no 2-cycle;

   (c) there are divergent orbits.

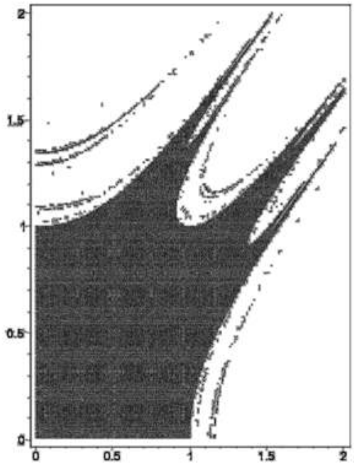


Figure 9.7. The region of convergence for φ.

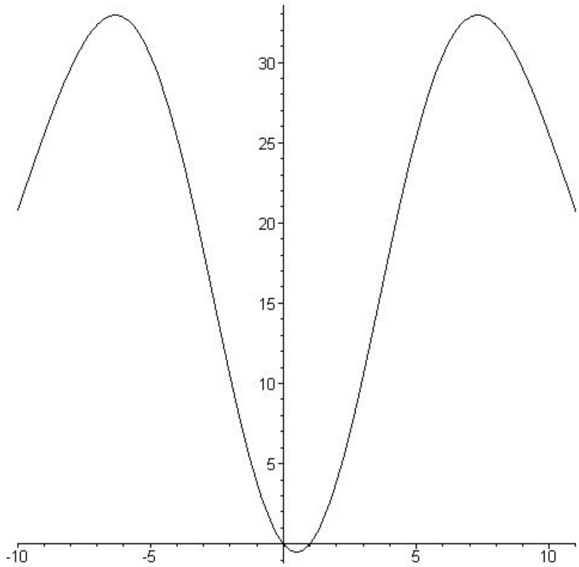


Figure 9.8. The symmetry of S/ζ.

It is instructive to plot the points for which the system appears to converge, as in Figure 9.7.

10. (Volume, surface area, and ζ.) Recall that the volume and surface area of the ball in d-dimensional space are given respectively by

$$V(d) := \frac{\pi^{d/2}}{\Gamma(d/2+1)} \quad \text{and} \quad S(d) := \frac{2\,\pi^{d/2}}{\Gamma(d/2)}.$$

   (a) Plot $V_\zeta := V/\zeta$ and $S_\zeta := S/\zeta$.

   (b) We observe, as Douglas S. Robertson did, that S_ζ appears symmetric about $z = 1/2$. This is illustrated in Figure 9.8.

   (c) Show that the symmetry

$$\frac{S(z)}{\zeta(z)} = \frac{S(1-z)}{\zeta(1-z)}$$

   is equivalent to Riemann's functional equation for ζ, namely

$$\pi^{-(1-z)/2}\Gamma\left(\frac{1-z}{2}\right)\zeta(1-z) = \pi^{-z/2}\Gamma\left(\frac{z}{2}\right)\zeta(z).$$

   (d) Use the duplication formula for Γ to derive a formula originally conjectured by Euler

$$\zeta(1-z) = 2^{1-z}\pi^{-z}\cos\left(\frac{z}{2}\right)\Gamma(z)\zeta(z).$$

11. Evaluate

$$\sum_{k=1}^{\infty}\sum_{j=1}^{\infty}\frac{H_j\,(H_{k+1}-1)}{kj\,(k+1)\,(j+k)},$$

where as before $H_k := \sum_{i=1}^{k} 1/i$.

Hint: The answer is a combination of $\zeta(2), \zeta(3), \zeta(5)$, and $\zeta(2)\zeta(3)$.

12. (A multi-dimensional binomial series.) We consider, following Benoit Cloitre, the series

$$B_N := \sum_{n_i,n_2,\ldots,n_N\geq 0} \frac{1}{\binom{2\sum_{i=1}^N n_i}{\sum_{i=1}^N n_i}}.$$

By computing the first two values exactly

$$B_1 := \frac{4}{3}+\frac{2}{9}\frac{\pi}{\sqrt{3}}, \quad B_2 := 2+\frac{4}{9}\frac{\pi}{\sqrt{3}},$$

and the next two via PSLQ

$$B_3 = 3+\frac{20}{27}\frac{\pi}{\sqrt{3}}, \quad B_4 = \frac{40}{9}+\frac{280}{243}\frac{\pi}{\sqrt{3}},$$

we discover that the values all appear to be of the form $B_N = a_N + b_N\,\pi/\sqrt{3}$ with well-structured, rational, positive coordinates. Given the binomial coefficients, it is reasonable to look for a two-term recurrence. Again integer relation methods apply, and we quickly identify the first few terms of the recursion

$$3(n+1)\,B_{n+2}-(7n+6)\,B_{n+1}+2(2n+1)\,B_n = 0. \tag{9.105}$$

(It is advisable to limit the number of terms one must sum to obtain sufficient digits of B_n.)

(a) Prove that (9.105) holds and so B_N is of the conjectured form.

(b) Determine a closed form for B_N.

(c) Explore

$$B_N(r,s) := \sum_{n_i,n_2,\ldots,n_N\geq 0}{}' \frac{1}{\left(\sum_{i=1}^N n_i\right)^r \binom{2\sum_{i=1}^N n_i}{\sum_{i=1}^N n_i}^s}$$

for $r,s = 1,2\ldots$.

13. (A Gaussian integer zeta function.) Evaluate in closed form

$$\zeta_G(N) := \sum_{\mathbb{Z}(i)}{}' \frac{1}{z^N} = \sum_{m,n}{}' \frac{1}{(m+in)^N}$$

for positive, even integer $N>1$. Here as always the primes denotes that summation avoids the pole at 0.

Hint: This is implicitly covered in [51, pp. 167–170] and in [211]. It relies on analysis of the *Weierstrass* $\wp$ *function*; see [1, Chapter 18]. We recall that

$$\wp(x) := \sum{}' \frac{1}{(2in+2im-x)^2} - \frac{1}{(2in+2im)^2}.$$

We then differentiate twice and extract the coefficients of $\zeta_G(2n)$. For N divisible by four, the sum is actually a rational multiple of powers of the invariants

$$g_2 = K\left(\frac{1}{\sqrt{2}}\right)^4 = \left(\frac{1}{4}\beta\left(\frac{1}{4}\right)\right)^4$$

and $g_3 = 0$. This is the so-called *lemniscate case* of $\wp$. Here $\beta(x) := B(x,x)$ is the central Beta-function.

(a) Show that the general formula for $N \geq 1$ is

$$\zeta_G(4N) = p_N \frac{\left\{2K\left(1/\sqrt{2}\right)\right\}^{4N}}{(4N-1)},$$

where $p_1 = 1/20$ and

$$p_N = \frac{3\sum_{m=1}^{N-1} p_m\, p_{N-m}}{(4N+1)(2N-3)},$$

for $N > 1$. The next three values are $p_2 = 1/1200$, $p_3 = 1/156000$, and $p_4 = 1/21216000$. The corresponding values of $q_N := 16^N p_N$ are

$$\frac{4}{5}, \frac{16}{75}, \frac{128}{4875}, \frac{256}{82875}.$$

Finally note that q_N satisfies the same recursion. This leads to the simple expression

$$\zeta_G(4N) = \frac{q_N}{4N-1} K\left(\frac{1}{\sqrt{2}}\right)^{4N},$$

where $q_1 = 16/5$ and for $n > 1$

$$q_N = \frac{3\sum_{m=1}^{N-1} q_m\, q_{N-m}}{(4N+1)(2N-3)}.$$

(b) Show that, for N congruent to 2 mod 4, the sum is

$$\zeta_G(4N+2) = \sum_{\mathbb{Z}(i)}{}' \frac{1}{z^{4N+2}} = 4\,\zeta(4N+2),$$

since

$$\begin{aligned} 2\sum_{m,n>0}{}' \frac{1}{z^{4N+2}} &= \sum_{m,n>0} \frac{(m+in)^{4n+2}}{(m^2+n^2)^{4N+2}} + \sum_{m,n>0} \frac{(n+im)^{4n+2}}{(m^2+n^2)^{4N+2}} \\ &= \sum_{m,n>0} \frac{\operatorname{Re}\left((m+in)^{4n+2} + (n+im)^{4n+2}\right)}{(m^2+n^2)^{4N+2}} = 0 \end{aligned}$$

as the terms cancel pairwise. If we observe that $\pi^2 = \beta(1/2)^2$, we may more uniformly write

$$\zeta_G(4N) = \frac{q_N}{(4N-1)4^{4N}}\,\beta(1/4)^{4N},$$

$$\zeta_G(4N+2) = \frac{b_{4N+2}\,2^{4N+1}}{(4N-1)(4N+2)!}\,\beta(1/2)^{4N+2},$$

where b_N is the Nth Bernoulli number. By contrast, it is easily seen that

$$\zeta_G(2N+1) = 0.$$

14. The generalized quantum sum is defined by

$$\mathscr{Y}(a,b,c) := \sum{}' \frac{1}{(z-a)(z-b)(z-c)}$$

with a,b,c fixed, but not on the lattice. Show that $\mathscr{Y}$ has a formal power series development in $\zeta_G(n)$ for even n, just by writing the summand as

$$1/z^3\,(1+a/z+a^2/z^2+\ldots)(1+b/z+b^2/z^2+\ldots)(1+c/z+c^2/z^2+\ldots).$$

For $|a|,|b|,|c| < 1$, this leads to

$$\mathscr{Y}(a,b,c) = \sum_{n=1}^{\infty} \pi_n(a,b,c)\,\zeta_G(2n+2),$$

where

$$\pi_n(a,b,c) := \sum_{k_1+k_2+k_3=n} a^{k_1} b^{k_2} c^{k_3}.$$

In particular, $\pi_n(a,a,a) = \binom{n}{2}\,a^3$. There is a corresponding expansion for more than three linear terms.

15. The following evaluation is given in [170] and used in several interesting applications.

Theorem 9.8. *For $0 < a < b$, if f is defined by the requirement that $f(x)^a - f(x)^b = x^a - x^b$ and f is decreasing, then*

$$-\int_0^1 \frac{\log f(x)}{x}\,dx = \frac{\pi^2}{3ab}. \tag{9.106}$$

The picture in Figure 9.9 shows how f is defined.

The proof is quite elaborate and relies on (i) a reduction to the case $b = 1$ and (ii) application of the following identity after splitting the integral in (9.106) at $1/(a+1)$.

(a) Prove that for $0 < x < 1/(a+1)$

$$G_a(1-x) := \sum_{n=1}^{\infty} \frac{\Gamma((a+1)n)}{\Gamma(an)}\,\frac{(x(1-x)^a)^n}{(na)\,n!} = -\log(1-x).$$

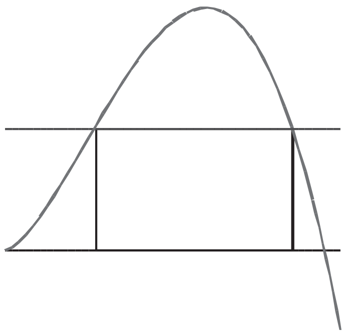


Figure 9.9. The construction of f.

(b) We request a geometric proof of (9.106). We do not know one.

(c) The function f can be determined explicitly in some cases:

(i) $(b = 2a)$ $f(x) = 3(1 - x^a)^{1/a}$.

(ii) $(b = 3a)$ $f(x) = 3(-x^a/2 + \sqrt{4 - 3x^{2a}})^{1/a}$.

(iii) $(2b = 3a)$ $f(x) = 3(-x^a/2 + +\sqrt{-3x^{2a} + 2x^a + 1})^{1/a}$.

16. Determine the limit of $\gamma_n := n \int_0^1 t^{n-1}\left((1+t)/2\right)^n dt$ as n goes to infinity.
Hint: It may help to show that the value $\gamma_n = {}_2\mathrm{F}_1\left(1, -n; n+1; 1/2\right)$.

17. (The number 1729 revisited.) Famously, G. H. Hardy while visiting Ramanujan in hospital remarked that his cab number 1729 was very uninteresting, to which Ramanujan replied that it was very interesting, being the smallest number expressible as the sum of two integer cubes in two distinct ways:

$$1729 = 10^3 + 9^3 = 12^3 + 1.$$

(a) Determine the second smallest number with this property, that is, with $r_3(n) = 2$.

(b) As Hirschhorn [168] observes, 1729 is also special in being a solution to $n = x^3 \pm 1$. Indeed, in the *Lost Notebook* Ramanujan states that the recursion for $u_n = (x_n, y_n, z_n)$,

$$u_{n+3} := 82\, u_{n+2} + 82\, u_{n+1} - u_n, \tag{9.107}$$

with initial conditions $u_1 := (9, 10, 12)$, $u_2 := (791, 812, 1010)$, and $u_3 := (65601, 67402, 83802)$, solves

$$x_n^3 + y_n^3 - z_n^3 = (-1)^{n+1}$$

for all (positive and negative) integer n. Thus, we have infinitely many near misses to Fermat's equation. For example, $u_{-1} = (-2, 2, 1)$ and

$$x_{12} = 12247547739697622322431,$$

$$y_{12} = 1258365789240770271600 2,$$

and

$$z_{12} = 1564554482733210829661 0.$$

(c) There is a 3×3 matrix M, with minimal polynomial $1 - 82t - 82t^2 + t^3$ and determinant -1, such that $u_n = M\,u_{n-1}$. We have

$$M := \begin{bmatrix} 63 & 68 & -104 \\ -80 & -85 & 131 \\ -64 & -67 & 104 \end{bmatrix} \text{ with } M^{-1} = \begin{bmatrix} 63 & 104 & -68 \\ 64 & 104 & -67 \\ 80 & 131 & -85 \end{bmatrix}.$$

(d) Try to prove that if $a^3 + b^3 - c^3 = \pm 1$, then $M(a,b,c) = (a',b',c')$ satisfies $a'^3 + b'^3 - c'^3 = \mp 1$.

(e) Failing that, begin with

$$\left(x^2 + 9x - 1\right)^3 + \left(2x^2 + 10\right)^3 = \left(x^2 - 7x - 9\right)^3 + \left(2x^2 + 4x + 12\right)^3.$$

Now replace x by v/u, multiply by u^6, and obtain the resulting homogeneous identity:

$$\left(10u^2 + 2v^2\right)^3 + \left(9u^2 + 7uv - v^2\right)^3 =$$
$$\left(12u^2 + 4uv + 2v^2\right)^3 + \left(u^2 - 9uv - v^2\right)^3.$$

(f) Check that the sequence $s_0 := 0, s_1 := 1$, and $s_{n+1} := 9s_n + s_{n-1}$ for all $n > 1$ satisfies $s_n^2 - 9s_n s_{n-1} - s_{n-1}^2 = (-1)^{n-1}$. Hence,

$$(9s_n^2 + 7s_n s_{n-1} - s_{n-1}^2, 10s_n^2 + 2s_{n-1}^3, 12s_n^2 + 4s_n s_{n-1} + 2s_{n-1}^2)$$

parameterizes the sequence (u_n).

18. (Cheating God somehow.) Consider that

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

is valid to 268 places, while

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

is valid to just 12 places. Both are actually *transcendental numbers*. Correspondingly, the *simple continued fractions* for $\tanh(\pi)$ and $\tanh\left(\frac{\pi}{2}\right)$ are respectively

$$[0, 1, \mathbf{267}, 4, 14, 1, 2, 1, 2, 2, 1, 2, 3, 8, 3, 1]$$

and

$$[0, 1, \mathbf{11}, 14, 4, 1, 1, 1, 3, 1, 295, 4, 4, 1, 5, 17, 7].$$

Bill Gosper describes how continued fractions let you "see" what a number is: "[I]t's completely astounding ... it looks like you are cheating God somehow."

19. (Coincidences do occur.) The approximations

$$\pi \approx \frac{3}{\sqrt{163}} \log(640320) \quad \text{and} \quad \pi \approx \sqrt{2}\,\frac{9801}{4412}$$

occur for deep number theoretic reasons—the first good to 15 places, the second to 8. By contrast,

$$e^{\pi} - \pi = \mathbf{19.999099979}189475768\ldots$$

most probably for no good reason. This seemed more bizarre on an eight digit calculator. Likewise, as spotted by Pierre Lanchon recently,

$$e = \overline{\mathbf{10.10110111111000010}}101000101100\ldots$$

and

$$\pi = 11.0010\overline{\mathbf{0100001111110110101}}01000\ldots.$$

have 19 bits agreeing in base two, with one reading left to right and the other right to left!

More extended coincidences are almost always contrived, such as those in Exercise 18 and in Exercise 10(c), and strong heuristics exist for believing results like the empirical ζ-function evaluation of (9.20). But recall our discussion of the cosine integrals in Chapter 8, and the famous *Skewes number*,

$$\int_2^x \frac{dt}{\log t} \geq \pi(x) \quad \text{with first known failure around } 10^{360},$$

and the *Merten's Conjecture*,

$$\left|\sum_{k=1}^{n} \mu(k)\right| \leq \sqrt{n} \quad \text{with first known failure around } 10^{110}.$$

Here μ is the *Möbius function*.

20. (Roman numeration.) Consider the following Roman fraction:

$$\mathrm{II} = \frac{\mathrm{XXII}}{\mathrm{VIII}}.$$

A Hungarian school contest asked for a movement of one symbol to make a true identity.

Answer. The proposers thought

$$\overline{\mathrm{II}} = \frac{\mathrm{XXII}}{\mathrm{VII}}.$$

21. For general integer N, determine the inverse of $M_1 := A + B - C$ and $M_2 := A + B + 2C$ when A, B, and C are $N \times N$ matrices with entries

```
A:=N->Matrix(N,N,(j,k)->(-1)^(k+1)*binomial(2*N-j,2*N-k));
B:=N->Matrix(N,N,(j,k)->(-1)^(k+1)*binomial(2*N-j,k-1));
C:=N->Matrix(N,N,(j,k)->(-1)^(k+1)*binomial(j-1,k-1));
```

Hint: $A^2 = C^2 = I$ and $B = CA$.

22. (Some convexity properties [230].) Examine the convexity and log-convexity properties of

$$s_k(x) := \sum_{k=0}^{N} \frac{x^k}{k!} \quad \text{and} \quad t_k(x) := e^x - \sum_{k=0}^{N} \frac{x^k}{k!},$$

as a function of $x > 0$, for $k = 1, 2, \ldots$.

23. (Two trigonometric inequalities [230].)

    (a) Show that

    $$\frac{4}{\pi}\frac{x}{x^2-1} \le \tan\left(\frac{\pi x}{2}\right) \le \frac{\pi}{2}\frac{x}{x^2-1},$$

    for $0 < x < 1$.

    (b) Show that

    $$\left(\frac{\sin x}{x}\right)^3 > \cos x,$$

    for $0 < x < \pi/2$.

    (c) In what sense are these best possible?

24. (Dyson's conjecture [253].) For nonnegative integers $a_1, a_2, \cdots, a_n$, determine the constant term of

$$\prod_{1 \le i \ne j \le n} \left(1 - \frac{x_i}{x_j}\right)^{a_j}.$$

Hint: The coefficient is

$$\frac{(a_1 + a_2 + \ldots + a_n)!}{a_1!a_2!\ldots a_n!}.$$

25. (Other chaos games.) Determine how to adjust the random fractal triangle of Chapter 8 to generate the hexagon in Figure 9.10 and like shapes.

Hint: Consult [117].

Figure 9.10. A random Sierpinski hexagon.

26. (Fourteen proofs of a result about tiling a rectangle.) [274,282]. Prove that whenever a rectangle is tiled by rectangles each of which has at least one integer side, then the ambient rectangle has at least one integer side.

27. "But, My Lord, being by you found out, I wonder nobody else found it out before, when, now known, it is so easy." Discoveries often have this feature. They may be

rapidly transformative as this account by Garry J. Tee (Auckland) makes clear. Immediately after the publication of Napier's *Miraculous Canon of Logarithms* (Edinburgh 1614), Briggs began teaching logarithms at Gresham College. He convinced the Honorable East India Company that they needed logarithms to enable their captains to navigate ships to India and return. The Honorable Company paid Edward Wright (Savilian Professor of Geometry at Oxford) to translate Napier's Latin text into English, and in 1615 Henry Briggs undertook the laborious journey from London to Edinburgh, taking the manuscript translation for checking by Napier. Briggs was acquainted with John Marr (or Mair), who was compass-maker and dial-maker to the kings James VI and Charles I. Marr witnessed that meeting, and he reported it to the prominent astrologist William Lilly (1602–1681), who was consulted by the Commonwealth Government about an auspicious date on which to execute King Charles I. Auckland City Library has a copy of "Mr Lilly's History of His Life and Times" (published 1715), with Marr's report of that meeting:

> I will acquaint you with one memorable story related unto me by Mr John Marr, an excellent mathematician and Geometer whom I conceive you remember. He was servant to King James and Charles. At first, when the Lord Napier of Merchiston made public his logarithms, Mr Briggs, then Reader of the Astronomy lecture at Gresham College in London, was so surprised with admiration of them that he could have no quietness in himself until he had seen that noble person, the Lord Merchiston, whose only invention they were. He acquaints Mr Marr herewith, who went into Scotland before Mr Briggs, purposely to be there when these so learned persons should meet. Mr Briggs appoints a certain day, when to meet in Edinburgh, but failing thereof, the Lord Napier was doubtful he would not come. It happened one day as John Marr and the Lord Napier were speaking of Mr Briggs; "Ah, John," says Merchiston, "Mr Briggs will not come now". At the very instant one knocks on his gate. John Marr hasted down, and it proved Mr Briggs to his great contentment. He brings Mr Briggs up into my Lord's chamber, where almost one quarter of an hour was spent, each beholding other almost with admiration, before one word was spoke. At last Mr Briggs began; *"My Lord, I have undertaken this long journey purposely to see your person, and to know by what engine of wit or ingenuity you came first to think of this most excellent help unto Astronomy, namely logarithms. But, My Lord, being by you found out (i.e. discovered), I wonder nobody else found it out before, when, now known, it is so easy*". He was nobly entertained by the Lord Napier, and every summer after that, during the Lord's being alive, this venerable man Mr Briggs went into Scotland purposely to visit him. These two persons were worthy men in their time, and yet the one, namely Lord Merchiston, was a great lover of Astrology; but Briggs the most satyrical man against it that was ever

> known. But the reason hereof I conceive was that Briggs was a severe Presbyterian, and wholly conversant with persons of that judgement; whereas the Lord Merchiston was a general scholar, and deeply read in all divine and human histories. This is the same Merchiston who made the most serious and learned exposition upon the *Revelation of St. John*, which is the best that ever yet appeared in the world.

Briggs and Napier independently invented decimal logarithms, and in 1615 Briggs agreed to compute tables of the new form of logarithms. He visited Napier again in 1616 and prepared to visit him again in 1617, but Napier died on April 4, 1617.

28. (Which sequence grows faster?) For $b > a > 0$ and $n \geq 0$, which sequence is ultimately larger: $a^{(b^n)}$ or $b^{(a^n)}$. When?

29. (What is eerie about this limit?) Define the sequence e_n by $e_1 = 0, e_2 = 1$, and $e_n = e_{n-1} + e_{n-2}/(n-2)$. What is the limit of n/e_n as n approaches infinity? What is the rate of convergence?

30. (Jeff Tupper's self-referent fact.) (What is it?) Graph the set of points (x, y) such that
$$\frac{1}{2} < \left\lfloor \operatorname{mod}\left(\left\lfloor \frac{y}{17} \right\rfloor 2^{-17\lfloor x \rfloor - \operatorname{mod}(\lfloor y \rfloor, 17)}, 2 \right) \right\rfloor$$
in the region $0 < x < 107$ and $N < y < N + 17$, where N is the following 541-digit integer:

960939379918958884971672962127852754715004339660129306651505
519271702802395266424689642842174350718121267153782770623355
993237280874144307891325963941337723487857735749823926629715
517173716995165232890538221612403238855866184013235585136048
828693337902491454229288667081096184496091705183454067827731
551705405381627380967602565625016981482083418783163849115590
225610003652351370343874461848378737238198224849863465033159
410054974700593138339226497249461751545728366702369745461014
6559979337985374831437868418065934222278983887229800007484047

The picture in Figure 9.11 shows what transpires.

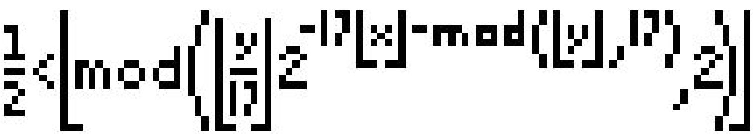


Figure 9.11. The answer is . . . .

31. Show that for $n = 1, 2, 3\ldots$

$$\frac{2}{\pi}\int_0^\infty \left(\frac{\sin x}{x}\right)^n dx = \frac{n}{2^{n-1}} \sum_{r=0}^{\lceil n/2\rceil - 1} (-1)^r \, \frac{(n-2r)^{n-1}}{(n-r)!\,r!}.$$

32. (Putnam Problem A6, 1999.) Suppose $u_1 = 1, u_2 = 2, u_3 = 24$, and

$$u_n = \frac{6\,u_{n-1}^2 u_{n-3} - 8\,u_{n-1} u_{n-2}^2}{u_{n-2} u_{n-3}}.$$

Show that u_n is always a multiple of n.

Hint: Determine the recursion for u_n/u_{n-1}.

33. Confirm the following Bernoulli number congruences for prime $p > 3$ [91]:

(a)

$$\sum_{k=1}^{p-1} \frac{1}{k} \equiv -\frac{p^2}{3} B_{p-3} \bmod p^3$$

(b)

$$\sum_{k=1}^{p-1} \frac{\sum_{j=1}^{k-1} 1/j}{k} \equiv -\frac{p}{3} B_{p-3} \bmod p^2$$

(c)

$$\sum_{k=1}^{p-1} \frac{1}{k^2} \equiv \frac{2p}{3} B_{p-3} \bmod p^2$$

(d)

$$\sum_{i+j+k=p} \frac{1}{ijk} \equiv -2 B_{p-3} \bmod p$$

34. (A generating function due to Hongwei Chen.) Prove that

$$\sum_{k=1}^{\infty} \sum_{j=1}^{k} \frac{1}{2j-1} x^{2k-1} = \frac{-\frac{1}{2}\log\left(\frac{1-x}{1+x}\right)}{1-x^2}, \tag{9.108}$$

$$\sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k} \frac{1}{2j-1}}{k} x^{2k} = \frac{1}{4}\log^2\left(\frac{1-x}{1+x}\right), \tag{9.109}$$

and so

$$\begin{aligned} \sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k} \frac{1}{2j-1}}{k^2} x^{2k} = {} & \frac{7}{4}\zeta(3) + \frac{1}{2}\log(x)\log^2\left(\frac{1-x}{1+x}\right) \\ & + \left\{\mathrm{Li}_2\left(\frac{1-x}{1+x}\right) - \mathrm{Li}_2\left(-\frac{1-x}{1+x}\right)\right\} \\ & \times \log\left(\frac{1-x}{1+x}\right) \\ & - \left\{\mathrm{Li}_3\left(\frac{1-x}{1+x}\right) - \mathrm{Li}_3\left(-\frac{1-x}{1+x}\right)\right\}. \end{aligned} \tag{9.110}$$

Hint: Reduce (9.110) to (9.109) and then to (9.108) by differentiating. Determine the constants of integration by taking limits at zero. Hence, evaluate sums such as $\sum_{k=1}^{\infty}\frac{(-1)^k}{k^2}\sum_{j=1}^{k}\frac{1}{2j-1}$ and $\sum_{k=1}^{\infty}\frac{1}{3^k k^2}\sum_{j=1}^{k}\frac{1}{2j-1}$.
Note that $\mathrm{Li}_n(y)-\mathrm{Li}_n(-y)=2\sum_{k=0}^{\infty}y^{2k+1}/(2k+1)^n$. A more systematic analysis of such *character Euler sums* is to be found in [71].

35. (A generating function due to Jorge Cimadev.) Show for $|x|<1$ that

$$\sum_{n=0}^{\infty}\frac{x^{n+1}\sum_{k=0}^{n}1/\binom{n}{k}}{n+1}=-2\,\frac{\log(1-x)}{2-x},$$

and deduce that

$$\sum_{n=0}^{\infty}\frac{x^{n+1}\sum_{k=0}^{n}1/\binom{n}{k}}{(n+1)^2}+2\sum_{n=0}^{\infty}\frac{(1-x)^{2n+1}}{(2n+1)^2}=\log(1-x)\log(2/x-1)+\frac{\pi^2}{4}.$$

Hence, obtain a closed form for series such as

$$\sum_{n=0}^{\infty}\frac{\sum_{k=0}^{n}1/\binom{n}{k}}{(n+1)^2\,2^{n+1}}.$$

36. (A final integral.) Evaluate

$$Z:=\int_0^1\int_0^1\frac{\log\left(\frac{y(1-y)}{z(1-z)}\right)}{y(1-y)-z(1-z)}\,dy\,dz$$

in closed form.

Hint: Use the change of variables $y(1-y)=s, z(1-z)=t$ to show that $Z=-2\int_0^1\frac{\log(1-s^2)\,\mathrm{arctanh}(s)}{s}\,ds=2.10359958052929\ldots$. Identify this constant numerically and prove your discovery [18].

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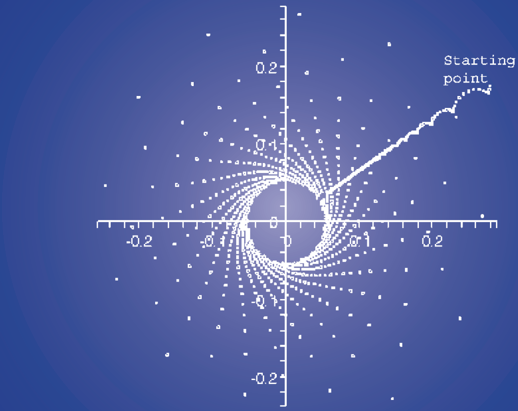

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