Experimental (Computational) Mathematics

and

Philosophical Implications

Based on the 2005 Clifford Lectures

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From the Sep. 12, 2005 issue From the Magazine I Innovators Chaitin's universal halting constant Posted Sunday, Sep. 04, 2005 It Doesn't Figure $\Omega = 0.0000010000010000100001000011101110$ The Omega Man 01100100111100010010011100 Online Edition By MICHAEL D. LEMONICK (Calude) 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."

Chaitin's idea centers on a number he calls **omega**, which he discovered in 1975 and which is much too complicated to explain here. (Chaitin's book Meta Math! The Quest for Omega, out this month, should help make omega clear.) Suffice it to say that the concept broadens two major discoveries of 20th century math: Gödel's incompleteness theorem, which says there will always be unprovable statements in any system of math, and Turing's halting problem, which says it's impossible to predict in advance whether a particular computer calculation can ever be finished.

Sounds like a nonevent in the real world, but it may not be. Cryptographers assume that their mathematically based encryption schemes are unbreakable. Oops. "If any of these people wake up at night and worry," says Chaitin, "I'm giving them theoretical justification."



Experimental Mathematics:

And Its Implications

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Elsewhere 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 M. Edwards, 2004)



AK Peters 2004

Talk Revised: 03–23–05

Two Scientific Quotations

Kurt Gödel overturned the mathematical apple cart entirely deductively, but he held quite different ideas about legitimate forms of mathematical reasoning:

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.*

and *Christof Koch* accurately captures scientific distaste for philosophizing:

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. (Christof Koch[†], 2004)

*Taken from an until then unpublished 1951 manuscript in his *Collected Works*, Volume III.

[†]In "Thinking About the Conscious Mind," a review of John R. Searle's *Mind. A Brief Introduction*, OUP 2004.

Three Mathematical Definitions

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* makes no immediate mention of proof, nor of the means of reasoning to be allowed. *Webster's Dictionary* 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 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.

I, like Gödel, and as I shall show many others, suggest that both should be openly entertained in mathematical discourse.

My Intentions in these Lectures

I aim to discuss Experimental Mathodology, its philosophy, history, current practice and proximate future, and using concrete accessible—entertaining I hope—examples, to explore implications for mathematics and for mathematical philosophy.

Thereby, to persuade you both of the power of mathematical experiment and that the traditional accounting of mathematical learning and research is largely an ahistorical caricature.

The four lectures are largely independent

The tour mirrors that from the recent books:

Jonathan M. Borwein and David H. Bailey, *Mathematics by Experiment: Plausible Reasoning in the 21st Century*; and with Roland Girgensohn, *Experimentation in Mathematics: Computational Paths to Discovery*, A.K. Peters, Natick, MA, 2004.

The Four Clifford Lectures

1. Plausible Reasoning in the 21st Century, I.

This first lecture will be a general introduction to

Experimental Mathematics, its Practice and its Philosophy.

It will reprise the sort of 'Experimental methodology' that David Bailey and I—among many others—have come to practice over the past two decades.*



Dalhousie-DRIVE

*All resources are available at www.experimentalmath.info.

2. Plausible Reasoning in the 21st Century, II.

The second lecture will focus on the differences between

Determining Truths or Proving Theorems.

We shall explore various of the tools available for deciding what to believe in mathematics, and—using accessible examples illustrate the rich experimental tool-box mathematicians can now have access to.



Dalhousie-DRIVE

3. Ten Computational Challenge Problems.

This lecture will make a more advanced analysis of the themes developed in Lectures 1 and 2. It will look at 'lists and challenges' and discuss *Ten Computational Mathematics Problems* including

$$\int_0^\infty \cos(2x) \prod_{n=1}^\infty \cos\left(\frac{x}{n}\right) \, dx \stackrel{?}{=} \frac{\pi}{8}.$$

This problem set was stimulated by Nick Trefethen's recent more numerical *SIAM 100 Digit, 100 Dollar Challenge*.*

Die ganze Zahl schuf der liebe Gott, alles Ubrige ist Menschenwerk. God made the integers, all else is the work of man. (Leopold Kronecker, 1823-1891)

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*The talk is based on an article to appear in the May 2005 *Notices of the AMS*, and related resources such as www.cs.dal.ca/~jborwein/digits.pdf.

4. Apéry-Like Identities for $\zeta(n)$.

The final lecture comprises a research level case study of generating functions for zeta functions. This lecture is based on past research with David Bradley and current research with David Bailey.

One example is:

$$\begin{aligned} \mathcal{Z}(x) &:= 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}(k^2 - x^2)} \prod_{n=1}^{k-1} \frac{4x^2 - n^2}{x^2 - n^2} \\ &= \sum_{n=1}^{\infty} \frac{1}{n^2 - x^2} \\ &\left[= \sum_{k=0}^{\infty} \zeta(2k+2) x^{2k} = \frac{1 - \pi x \cot(\pi x)}{2x^2} \right]. \end{aligned}$$

Note that with x = 0 this recovers

$$3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}k^2} = \sum_{n=1}^{\infty} \frac{1}{n^2} = \zeta(2).$$

Experiments and Implications

I shall talk broadly about experimental and heuristic mathematics, giving accessible, primarily visual and symbolic, examples. The typographic to digital culture shift is vexing in math, viz:

- There is still no truly satisfactory way of displaying mathematics on the web
- We respect authority* but value authorship deeply
- And we care more about the reliability of our literature than does any other science

While the traditional central role of proof in mathematics is arguably under siege, the opportunities are enormous.

• Via examples, I intend to ask:

*Judith Grabiner, "Newton, Maclaurin, and the Authority of Mathematics," MAA, December 2004

MY 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?

DEWEY on HABITS

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. ··· 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)

* The Influence of Darwin on Philosophy, 1910. Dewey knew 'Comrade Van' in Mexico.

- Why I am a computer assisted fallibilist/social constructivist"
- ★ Rigour (proof) follows Reason (discovery)
- ★ Excessive focus on rigour drove us away from our wellsprings
 - Many ideas are false. Not all truths are provable. Not all provable truths are worth proving ...
- ★ Near certainly is often as good as it gets— intellectual context (community) matters
 - Complex human proofs are fraught with error (FLT, simple groups, ···)
- ★ Modern computational tools dramatically change the nature of available evidence

► Many of my more sophisticated examples originate in the boundary between mathematical physics and number theory and involve the ζ -function, $\zeta(n) = \sum_{k=1}^{\infty} \frac{1}{k^n}$, and its relatives.

They often rely on the sophisticated use of *Integer Relations Algorithms* — recently ranked among the 'top ten' algorithms of the century. Integer Relation methods were first discovered by our colleague **Helaman Ferguson** the mathematical sculptor.

In 2000, Sullivan and Dongarra wrote "Great algorithms are the poetry of computation," 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".*

- Newton's method was apparently ruled ineligible for consideration.
- *From "Random Samples", *Science* page 799, February 4, 2000. The full article appeared in the January/February 2000 issue of *Computing in Science & Engineering*. Dave Bailey wrote the description of 'PSLQ'.

The 20th century's Top Ten

- #1. 1946: The Metropolis Algorithm for Monte Carlo. Through the use of random processes, this algorithm offers an efficient way to stumble toward answers to problems that are too complicated to solve exactly.
- #2. 1947: Simplex Method for Linear Programming. An elegant solution to a common problem in planning and decision-making.
- #3. 1950: Krylov Subspace Iteration Method. A technique for rapidly solving the linear equations that abound in scientific computation.
- #4. 1951: The Decompositional Approach to Matrix Computations. A suite of techniques for numerical linear algebra.
- #5. 1957: The Fortran Optimizing Compiler. Turns high-level code into efficient computer-readable code.

- #6. 1959: QR Algorithm for Computing Eigenvalues. Another crucial matrix operation made swift and practical.
- #7. 1962: Quicksort Algorithms for Sorting. For the efficient handling of large databases.
- #8. 1965: Fast Fourier Transform. Perhaps the most ubiquitous algorithm in use today, it breaks down waveforms (like sound) into periodic components.
- #9. 1977: **Integer Relation Detection**. A fast method for spotting simple equations satisfied by collections of seemingly unrelated numbers.
- #10. 1987: Fast Multipole Method. A breakthrough in dealing with the complexity of n-body calculations, applied in problems ranging from celestial mechanics to protein folding.

Eight of these appeared in the first two decades of serious computing. Most are multiply embedded in every major mathematical computing package.

FOUR FORMS of EXPERIMENTS

We should discuss what Experiments are!

♣ <u>Kantian</u> examples: generating "the classical non-Euclidean geometries (hyperbolic, elliptic) by replacing Euclid's axiom of parallels (or something equivalent to it) with alternative forms."

♦ The <u>Baconian</u> experiment is a contrived as opposed to a natural happening, it "is the consequence of 'trying things out' or even of merely messing about."

 \heartsuit <u>Aristotelian</u> 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." ♠ The most important is <u>Galilean</u>: "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 only form which will make Experimental Mathematics a serious enterprise.





A Julia set From Peter Medawar (1915–87) *Advice to a Young Scientist* (1979)

A PARAPHRASE of HERSH

In any event mathematics is and will remain a uniquely human undertaking. Indeed Reuben Hersh's arguments for a humanist philosophy of mathematics, as paraphrased below, become more convincing in our 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.

2. Mathematical knowledge is fallible. As in science, mathematics can advance by making mistakes and then correcting or even recorrecting 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 (1997), 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 post-modern 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.

 "Fresh Breezes in the Philosophy of Mathematics", MAA Monthly, Aug 1995, 589–594.



A 2-coloring?

A PARAPHRASE of ERNEST

The idea that what is accepted as mathematical knowledge is, *to some degree*, dependent upon a community's methods of knowledge acceptance is central to the *social constructivist* school of mathematical philosophy.

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

Associated most notably with the writings of Paul Ernest* social constructivism seeks to define mathematical knowledge and epistemology through the social structure and interactions of the mathematical community and society as a whole.

DISCLAIMER: Social Constructivism is not Cultural Relativism

*In Social Constructivism As a Philosophy of Mathematics, Ernest, an English Mathematician and Professor in the Philosophy of Mathematics Education, carefully traces the intellectual pedigree for his thesis, a pedigree that encompasses the writings of Wittgenstein, Lakatos, Davis, and Hersh among others.

A NEW PROOF $\sqrt{2}$ is IRRATIONAL

One can find new insights in the oldest areas:

• Here is Tom Apostol's lovely new graphical proof* of the irrationality of $\sqrt{2}$. I like very much that this was published in the present millennium.



Root two is irrational (static and self-similar pictures)



**MAA Monthly*, November 2000, 241–242.

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

Circumscribe a circle of radius one side and construct the tangent on the hypotenuse [See picture].

Repeating the process once yields a yet smaller such triangle in the same orientation as the initial one.

The *smaller* triangle again has integer sidesQED

Note the philosophical transitions.

- Reductio ad absurdum \Rightarrow minimal configuration
- Euclidean geometry \Rightarrow Dynamic geometry

I. Revolutions

By 1948, the Marxist-Leninist ideas about the proletariat and its political capacity seemed more and more to me to disagree with reality ... I pondered my doubts, and for several years the study of mathematics was all that allowed me to preserve my inner equilibrium. Bolshevik ideology was, for me, in ruins. I had to build another life.

Jean Van Heijenoort (1913-1986) With Trotsky in Exile, in Anita Feferman's From Trotsky to Gödel



• Dewey ran Trotsky's 'treason trial' in Mexico

II. It's Obvious ...

Aspray: Since you both [Kleene and Rosser] had close associations with Church, I was wondering if you could tell me something about him. What was his wider mathematical training and interests? What were his research habits? I understood he kept rather unusual working hours. How was he as a lecturer? As a thesis director?

Rosser: In his lectures he was painstakingly careful. There was a story that went the rounds. *If Church said it's obvious, then everybody saw it a half hour ago. If Weyl says it's obvious, von Neumann can prove it. If Lefschetz says it's obvious, it's false.**

*One of several versions of this anecdote in *The Princeton Mathematics Community in the 1930s*. This one in Transcript Number 23 (**PMC23**)

III. The Evil of Bourbaki

"There is a story told of the mathematician Claude Chevalley (1909–84), who, as a true Bourbaki, was extremely opposed to the use of images in geometric reasoning.



He is said to have been giving a very abstract and algebraic lecture when he got stuck. After a moment of pondering, he turned to the blackboard, and, trying to hide what he was doing, drew a little diagram, looked at it for a moment, then quickly erased it, and turned back to the audience and proceeded with the lecture....

...The computer offers those less expert, and less stubborn than Chevalley, access to the kinds of images that could only be imagined in the heads of the most gifted mathematicians, \dots "^a (Nathalie Sinclair)

^aChapter in *Making the Connection: Research and Practice in Undergraduate Mathematics*, MAA Notes, 2004 in Press.

IV. The Historical Record

And it is one of the ironies of this entire field that were you to write a history of ideas in the whole of DNA, simply from the documented information as it exists in the literature - that is, a kind of Hegelian history of ideas - you would certainly say that Watson and Crick depended on Von Neumann, because von Neumann essentially tells you how it's done.

But of course no one knew anything about the other. It's a great paradox to me that this connection was not seen. Of course, all this leads to a real distrust about what historians of science say, especially those of the history of ideas.* (Sidney Brenner)

*The 2002 Nobelist talking about von Neumann's essay on The General and Logical Theory of Automata on pages 35– 36 of My life in Science as told to Lewis Wolpert.

POLYA and HEURISTICS

"[I]ntuition comes to us much earlier and with much less outside influence than formal arguments which we cannot really understand unless we have reached a relatively high level of logical experience and sophistication."* (George Polya)



Scatter-plot discovery of a cardioid

*In Mathematical Discovery: On Understanding, Learning and Teaching Problem Solving, 1968.

Polya on Picture-writing



Polya's illustration of the change solution*

Polya, in a 1956 American Mathematical Monthly article provided three provoking examples of converting pictorial representations of problems into generating function solutions. We discuss the first one.

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

*Illustration courtesy Mathematical Association of America

This leads to the (US currency) generating function

$$\sum_{k\geq 0} P_k x^k = \frac{1}{(1-x)(1-x^5)(1-x^{10})(1-x^{25})(1-x^{50})}$$

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

to obtain $P_{100} = 292$ (243 for Canadian currency, which lacks a 50 cent piece but has a dollar coin in common circulation).

• Polya's diagram is shown in the Figure

• To see why, we use geometric series and consider the so called *ordinary generating function*

$$\frac{1}{1-x^{10}} = 1 + x^{10} + x^{20} + x^{30} + \cdots$$

for dimes and

$$\frac{1}{1 - x^{25}} = 1 + x^{25} + x^{50} + x^{75} + \cdots$$

for quarters etc.

• We multiply these two together and compare coefficients

$$\frac{1}{1-x^{10}}\frac{1}{1-x^{25}} = 1+x^{10}+x^{20}+x^{25} + x^{30}+x^{35}+x^{40}+x^{45} + 2x^{50}+x^{55}+2x^{60}+\cdots$$

We argue that the *coefficient* of x^{60} on the right is precisely the number of ways of making 60 cents out of identical dimes and quarters.

- This is easy to check with a handful of change or a calculator, The general question with more denominations is handled similarly.
- I leave it open whether it is easier to decode the generating function from the picture or vice versa
 - in any event, symbolic and graphic experiment provide abundant and mutual reinforcement and assistance in concept formation.

"In the first place, the beginner must be convinced that proofs deserve to be studied, that they have a purpose, that they are interesting." (George Polya)

While by 'beginner' George Polya intended young school students, I suggest this is equally true of anyone engaging for the first time with an unfamiliar topic in mathematics.

Our MOTIVATION and GOALS

INSIGHT – demands speed \equiv **micro-parallelism**

- For rapid verification.
- For validation; proofs and refutations; "monster barring".
- ★ What is "easy" changes: HPC & HPN blur, merging disciplines and collaborators — democratizing math but challenging authenticity.
 - **Parallelism** \equiv more space, speed & stuff.
 - Exact ≡ hybrid ≡ symbolic '+' numeric (Maple meets NAG, Matlab calls Maple).
 - In analysis, algebra, geometry & topology.
... Moreover

- Towards an Experimental Mathodology— philosophy and practice.
- Intuition is acquired mesh computation and mathematics.
- Visualization 3 is a lot of dimensions.
- "Monster-barring" (Lakatos) and "Caging" (JMB):
 - <u>randomized checks</u>: equations, linear algebra, primality.
 - graphic checks: equalities, inequalities, areas.

... Graphic Checks

- Comparing $y y^2$ and $y^2 y^4$ to $-y^2 \ln(y)$ for 0 < y < 1 pictorially is a much more rapid way to divine which is larger than traditional analytic methods.
- It is clear that in the later case they cross, it is futile to try to prove one majorizes the other. In the first case, evidence is provided to motivate a proof.

Graphical comparison of $y - y^2$ and $y^2 - y^4$ to $-y^2 \ln(y)$ (red)

MINIMAL POLYNOMIALS of MATRICES

Consider matrices A, B, C, M:

$$A := \left[(-1)^{k+1} \binom{2n-j}{2n-k} \right], \quad B := \left[(-1)^{k+1} \binom{2n-j}{k-1} \right]$$
$$C := \left[(-1)^{k+1} \binom{j-1}{k-1} \right]$$
$$(k, j = 1, \dots, n) \text{ and set}$$

$$M := A + B - C$$

• In work on *Euler Sums* we needed to prove *M* invertible: actually

$$M^{-1} = \frac{M+I}{2}$$

• The key is discovering

$$A^{2} = C^{2} = I$$

$$B^{2} = CA, \quad AC = B.$$
(2)

 \therefore The group generated by A, B, C is S_3

 ◇ Once discovered, the combinatorial proof of this is routine – for a human or a computer ('A = B', Wilf-Zeilberger).

One now easily shows using (2)

$$M^2 + M = 2I$$

as formal algebra since M = A + B - C.

• In truth I started in Maple with cases of

'minpoly(M, x)'

and then emboldened I typed

'minpoly(B, x)'...

- Random matrices have full degree minimal polynomials.
- Jordan Forms uncover Spectral Abscissas.

OUR EXPERIMENTAL MATHODOLOGY

- 1. Gaining *insight* and intuition
- 2. Discovering new *patterns* and relationships
- 3. *Graphing* to expose math principles
- 4. Testing and especially *falsifying* conjectures
- 5. Exploring a possible result to see if it *merits* formal proof
- 6. Suggesting approaches for *formal proof*
- 7. Computing replacing lengthy hand derivations
- 8. Confirming analytically derived results

A BRIEF HISTORY OF RIGOUR

- Greeks: trisection, circle squaring, cube doubling and $\sqrt{2}$
- Newton and Leibniz: fluxions/infinitesimals
- Cauchy and Fourier: limits and continuity
- Frege and Russell, Gödel and Turing: paradoxes and types, proof and truth
- ENIAC and COQ: verification and validation



For continuous functions Fourier series need not converge: in 1810, 1860 or 1910?

THE PHILOSOPHIES OF RIGOUR

- Everyman: Platonism—stuff exists (1936)
- Hilbert: Formalism—math is invented; formal symbolic games without meaning
- Brouwer: Intuitionism-—many variants; ('embodied cognition')
- Bishop: Constructivism—tell me how big; (not 'social constructivism')
- \mho Last two deny *excluded middle*: $A \lor \tilde{A}$ and resonate with computer science—as does some of formalism.
- \equiv Absolutism versus Fallibilism.

SOME SELF PROMOTION

 Today Experimental Mathematics is being discussed quite widely

A Digital Slice of Pi

THE NEW WAY TO DO PURE MATH: EXPERIMENTALLY BY W. WAYT GIBBS

ne of the greatest ironies of the in-RER formation technology revolution is that while the computer was conceived and born in the field of pure mathematics, through the genius of giants such as John von Neumann and Alan Turing, until recently this marvelous technology had only a minor impact within the field that gave it birth." So begins Experimentation in Mathematics, a book by Jonathan M. Borwein and David H. Bailey due out in September that documents how all that has begun to change. Computers, once looked on by mathematical researchers with disdain as mere calculators, have gained enough power to enable an entirely new way to make fundamental discoveries: by running experiments and observing what happens.

The first clear evidence of this shift emerged in 1996. Bailey, who is chief technologist at the National Energy Research Sci-

www.sciam.com

entific Computing Center in Berkeley, Calif., and several colleagues developed a computer program that could uncover integer relations among long chains of real numbers. It was a problem that had long vexed

mathematicians. Euclid discovered the first integer relation scheme—a way to work out the greatest common divisor of any two integers—around 300 B.C. But it wasn't until 1977 that Helaman Ferguson and Rodney W. Forcade at last found a method to detect relations among an arbitrarily large set of numbers. Building on that work, in 1995 Bailey's group turned its computers loose on some of the fundamental constants of math, such as log 2 and pi.

To the researchers' great surprise, after months of calculations the machines came up with novel formulas for these and other nat-



COMPUTER RENDERINGS of mathematical constructs can

reveal hidden structure. The bands of color that appear in this plot of all solutions to a certain class of polynomials (specifically, those of the form $\pm 1 \pm x \pm x^2 \pm x^3 \pm ... \pm x^n = 0$, up to n = 18) have yet to be explained by conventional analysis.

MATH LAB

Computer experiments are transforming mathematics

BY ERICA KLARREICH

any people regard mathematics as the crown jewel of the sciences. Yet math has historically lacked one of the defining trappings of science: laboratory equipment. Physicists have their particle accelerators; biologists, their electron microscopes; and astronomers, their telescopes. Mathematics, by contrast, concerns not the physical landscape but an idealized, abstract world. For exploring that world, mathematicians have traditionally had only their intuition.

Now, computers are starting to give mathematicians the lab

instrument that they have been missing. Sophisticated software is enabling researchers to travel further and deeper into the mathematical universe. They're calculating the number pi with mind-boggling precision, for instance, or discovering patterns in the contours of beautiful, infinite chains of spheres that arise out of the geometry of knots.

Experiments in the computer lab are leading mathematicians to discoveries and insights that they might never have reached by traditional means. "Pretty much every [mathematical] field has been transformed by it," says Richard Crandall, a mathematician at Reed College in Portland, Ore. "Instead of just being a number-crunching tool, the computer is becoming more like a garden shovel that turns over rocks, and you find things underneath."

At the same time, the new work is raising unsettling questions about how to regard experimental results



UNSOLVED MYSTERIES — A computer experiment produced this plot of all the solutions to a collection of simple equations in 2001. Mathematicians are still trying to account for its many features.

"I have some of the excitement that Leonardo of Pisa must have felt when he encountered Arabic arithmetic. It suddenly made certain calculations flabbergastingly easy," Borwein says. "That's what I think is happening with computer experimentation today."

EXPERIMENTERS OF OLD In one sense, math experiments are nothing new. Despite their field's reputation as a purely deductive science, the great mathematicians over the centuries have never limited themselves to formal reasoning and proof.

For instance, in 1666, sheer curiosity and love of numbers led Isaac Newton to calculate directly the first 16 digits of the number pi, later writing, "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."

Carl Friedrich Gauss, one of the towering figures of 19th-cen-

tury mathematics, habitually discovered new mathematical results by experimenting with numbers and looking for patterns. When Gauss was a teenager, for instance, his experiments led him to one of the most important conjectures in the history of number theory: that the number of prime numbers less than a number x is roughly equal to xdivided by the logarithm of x.

Gauss often discovered results experimentally long before he could prove them formally. Once, he complained, "I have the result, but I do not yet know how to get it."

In the case of the prime number theorem, Gauss later refined his conjecture but never did figure out how to prove it. It took more than a century for mathematicians to come up with a proof.

Like today's mathematicians, math experimenters in the late 19th century used computers—but in those days, the word referred to people with a special facility for calcu-

From Science News April 2004

4. 22. 5



STRAIGHT CIRCLES — When mathematicians Colin Adams and Eric Schoenfeld created this image while playing with the computer program Snappea last year, they were stunned to see perfectly straight chains of spheres. The observation led them to an unexpected discovery about knots.

A Discovery in SnapPea

Bailey and Jonathan Borwein advance the controversial thesis that mathematics should move toward a more empirical approach. In it, formal proof would not be the only acceptable way to establish mathematical knowledge.

Mathematicians, Bailey and Borwein argue, should be free to work more like other scientists do, developing hypotheses through

experimentation and then testing them in further experiments. Formal proof is still the ideal, they say, but it is not the only path to mathematical truth.

"When I started school, I thought mathematics was about proofs, but now I think it's about having secure mathematical knowledge," Borwein says. "We claim that's not the same thing."

Bailey and Borwein point out that mathematical proofs can run to hundreds of pages and require such specialized knowledge that only a few people are capable of reading and judging them. "One thing that's happening is you can discover many more things than you can explain."

- JONATHAN BORWEIN DALHOUSIE UNIVERSITY

"We feel that in many cases, computations constitute very strong evidence, evidence that is at least as compelling as some of the more complex formal proofs in the literature," Bailey and Borwein say in *Mathematics by Experiment*.

CONCLUSION

Serving a Silicon Master

Mathematics by Experiment: Plausible Reasoning in the 21st Century. Jonathan Borwein and David Bailey. x + 288 pp. A K Peters, 2004. \$45.

Experimentation in Mathematics: Computational Paths to Discovery. Jonathan Borwein, David Bailey and Roland Girgensohn. x + 357 pp. A K Peters, 2004. \$49.

O nce upon a time, in ancient Greece, science was platonic and *a priori*. The Sun revolved around the Earth in a perfect circle, because the circle is such a perfect figure; there were four elements, because four is such a nice number, and so forth. Then along came Bacon, Boyle, Galileo, Kepler, Lavoisier, Newton and their buddies, and revolutionized science, making it experimental and empirical.

But math remains *a priori* and platonic to this day. Kant even went to excruciating lengths to "show" that geometry, although synthetic, is nevertheless *a priori*. Sure, all mathematicians, great and small, conducted experiments (until recently, using paper and pencil), but they kept their diaries and notebooks well hidden in the closet.

But stand by for a paradigm shift: Thanks to Its Omnipotence the Computer, math—that last stronghold of dear Plato—is becoming (overtly!) experimental, *a posteriori* and even contingent.

But what are poor pure mathematicians to do? Their professional weltanschauung—in other words, their philosophy—and more important, their working habits—in other words, their methodology—never prepared them for serving this new silicon master. Some of them, like the conceptual genius Alexander Grothendieck, even consider the computer (seriously!) the devil. But although many pure mathematicians strongly dislike and mistrust read both Mathematics by Experiment and Experimentation in Mathematics. Traditionalists may get annoyed, since the authors (Jonathan Borwein, David Bailey and Roland Girgensohn) don't make any bones about "math by experiment" being truly a paradigm shift. They even dedicate a whole section to the Kuhnian notion of paradigm shift, quoting Max Planck ("the transfer of allegiance from paradigm to paradigm is a conversion experience that cannot be forced") to make the point that we can't hasten acceptance of the new perspective, we can only be patient and wait for the old guard to die.

These are such fun books to read! Actually, calling them *books* does not do mathematician.

One of the many highlights is a detailed behind-the-scenes account of the discovery of the amazing Borwein-Bailey-Plouffe (BBP) formula for π :

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

(By the way, the Bailey is David, but the Borwein is Jonathan's brother Peter. Simon Plouffe, a latter-day Ramanujan, is the webmaster of the celebrated Inverse Symbolic Calculator site.)

The BBP formula allows one to compute the billion-and-first digit of π (in base 2) without computing the first billion digits. It was discovered with the aid



This figure plots all roots of polynomials, β_{N_r} with coefficients in {0, 1, -1} up to degree N=18. The zeroes are colored by their local density normalized to the range of densities, from red (low) to yellow (high). The fractal structures and holes around the roots come in different shapes and have precise locations. From *Experimentation in Mathematics*.

182 American Scientist, Volume 93

From American Scientist, March 2005

In the next Lecture we will return to these themes more mathematically. **Experimental Mathematics**:

Finding and Proving Things

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2005 Clifford Lecture II

Tulane, March 31–April 2, 2005

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



AK Peters 2004

DALHOUSIE UNIVERSITY

Inspiring Minds

Talk Revised: 03–20–05

The second lecture will focus on the differences between *Determining Truths or Proving Theorems*.

We shall explore various of the tools available for deciding what to believe in mathematics, and—using accessible examples illustrate the rich experimental tool-box mathematicians can now have access to.



The modulus of $\zeta(1/2 + it)$ —on the critical line

★ Let us start with some $T_EX...$

An Inverse Symbolic Discovery

Donald Knuth* asked for a closed form evaluation of:

$$\sum_{k=1}^{\infty} \left\{ \frac{k^k}{k! \, e^k} - \frac{1}{\sqrt{2 \pi \, k}} \right\} = -0.084069508727655\dots$$

- 2000 CE. It is easy to compute 20 or 200 digits of this sum
- ∠ The 'smart lookup' facility in the Inverse Symbolic Calculator[†] rapidly 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 laptop confirms to 100 places in under 6 seconds and to 500 in 40 seconds.

Arguably we are done.

*Posed as *MAA Problem* 10832, November 2002. †At www.cecm.sfu.ca/projects/ISC/ISCmain.html

A Fuller Account and a Proof

10832. Donald E. Knuth, Stanford University, Stanford, CA. Evaluate

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

1. A very rapid Maple computation yielded

 $-0.08406950872765600\ldots$

as the first 16 digits of the sum.

2. The *Inverse Symbolic Calculator* has a 'smart lookup' feature^{*} which replied that this was probably $-\frac{2}{3} - \zeta\left(\frac{1}{2}\right)/\sqrt{2\pi}$.

3. Ample experimental confirmation was provided by checking this to 50 digits. Thus within minutes we *knew* the answer.

4. As to why? **A clue** was provided by the surprising speed with which *Maple* computed the slowly convergent infinite sum.

*Alternatively, a sufficiently robust integer relation finder could be used.

 The package clearly knew something the user did not. Peering under the covers revealed that it was using the LambertW function, W, which is the inverse of w = z exp(z).*

5. The presence of $\zeta(1/2)$ and standard Euler-MacLaurin techniques, using Stirling's formula (as might be anticipated from the question), led to

$$\sum_{k=1}^{\infty} \left(\frac{1}{\sqrt{2\pi k}} - \frac{1}{\sqrt{2}} \frac{\left(\frac{1}{2}\right)_{k-1}}{(k-1)!} \right) = \frac{\zeta\left(\frac{1}{2}\right)}{\sqrt{2\pi}}, \qquad (1)$$

where the binomial coefficients in (1) are those of

$$\frac{1}{\sqrt{2-2\,z}}.$$

 \checkmark Now, (1) is a formula *Maple* can 'prove':

*A search in 2000 (2005) for "Lambert W" on *MathSciNet* provided 9 (25) references – all since 1997 when the function appears named for the first time in *Maple* and *Mathematica*.

6. It remains to show

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

7. Guided by the presence of W, and its series

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

an appeal to Abel's limit theorem lets one deduce the need to evaluate

$$\lim_{z \to 1} \left(\frac{d}{dz} \mathsf{W} \left(-\frac{z}{e} \right) + \frac{1}{\sqrt{2 - 2z}} \right) = \frac{2}{3}.$$
 (3)

 \square

 \checkmark Again Maple happily does know (3).

- Of course, this all took a *fair* amount of human mediation and insight.
- Less if Maple had been taught to recognize W from its series.

In the same vein ...

Consider the following two *Euler sum identities* both discovered heuristically.

Both merit quite firm belief—more so than many proofs.

Why?

• Only the first warrants significant effort being exerted for its proof.

Why and Why Not?





"Lisez Euler, lisez Euler

"Lisez Euler, lisez Euler, c'est notre maitre a tous." Goldbach precisely formulated by letter the series which sparked Euler's further investigations into what would become known as the *Zetafunction*.

• These investigations were apparently due to a serendipitous mistake.

Euler wrote back:

When I recently considered further the indicated sums of the last two series in my previous letter, I realized immediately that the same series arose due to a mere writing error, from which indeed the saying goes, "Had one not erred, one would have achieved less." (Si non errasset, fecerat ille minus).*

*Translation thanks to Martin Matmüller, scientific collaborator of Euler's *Opera Omnia*, vol. IVA4, Birkhäuser Verlag.

A FIRST MULTIPLE ZETA VALUE

Euler sums or *MZVs* are a wonderful generalization of the classical ζ function.

For natural numbers

$$\zeta(i_1, i_2, \dots, i_k) := \sum_{n_1 > n_2 > \dot{n}_k > 0} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}}$$

 \diamond Thus $\zeta(a) = \sum_{n \ge 1} n^{-a}$ is as before and

$$\zeta(a,b) = \sum_{n=1}^{\infty} \frac{1 + \frac{1}{2^b} + \dots + \frac{1}{(n-1)^b}}{n^a}$$

 \checkmark k is the sum's *depth* and $i_1 + i_2 + \cdots + i_k$ is its *weight*.

• This clearly extends to alternating and character sums.

 MZV's satisfy many striking identities, of which the simplest are

$$\zeta(2,1) = \zeta(3), \qquad 4\zeta(3,1) = \zeta(4).$$

- MZV's have found interesting interpretations in high energy physics, knot theory, combinatorics
 ...
- ✓ Euler found and partially proved theorems on reducibility of depth 2 to depth 1 ζ 's

- Goldbach's letter conjectured

$$\zeta(3,1) + \zeta(4) = \pi^4/72.$$

- $\zeta(6,2)$ is the lowest weight 'irreducible'
- ✓ High precision fast ζ-convolution (see EZFace/Java) allows use of integer relation methods and leads to important dimensional (reducibility) conjectures and amazing identities.

A Striking CONJECTURE open for all n > 2 is:

$$8^n \zeta(\{-2,1\}_n) \stackrel{?}{=} \zeta(\{2,1\}_n)$$

There is abundant evidence amassed since it was found in 1996.

- © For example, very recently Petr Lisonek checked the first 85 cases to 1000 places in about 41 HP hours with only the *expected error*. And N=163 was confirmed in ten hours.
 - This is the *only* identification of its type of an Euler sum with a distinct MZV.
 - Can even just the case n = 2 be proven symbolically as is the case for n = 1?

II. A CHARACTER EULER SUM

Let

$$[2b, -3](s, t) := \sum_{n > m > 0} \frac{(-1)^{n-1}}{n^s} \frac{\chi_3(m)}{m^t},$$

where χ_3 is the character modulo 3.

Then

[2b, -3](2N+1, 1)

$$= \frac{L_{-3}(2N+2)}{4^{1+N}} - \frac{1+4^{-N}}{2}L_{-3}(2N+1)\log(3)$$

+
$$\sum_{k=1}^{N} \frac{1-3^{-2N+2k}}{2}L_{-3}(2N-2k+2)\alpha(2k)$$

-
$$\sum_{k=1}^{N} \frac{1-9^{-k}}{1-4^{-k}} \frac{1+4^{-N+k}}{2}L_{-3}(2N-2k+1)\alpha(2k+1)$$

-
$$2L_{-3}(1)\alpha(2N+1).$$

✓ Here α is the alternating zeta function and L₋₃ is the primitive L-series modulo 3.

\checkmark One first evaluates such sums as integrals

COINCIDENCE or FRAUD

• Coincidences do occur

The approximations

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

and

$$\pi \approx \sqrt{2} \frac{9801}{4412}$$

occur for deep number theoretic reasons—the first good to 15 places, the second to eight

By contrast

 $e^{\pi} - \pi = 19.999099979189475768...$

most probably for no good reason.

✓ This seemed more bizarre on an eight digit calculator Likewise, as spotted by Pierre Lanchon recently

$e = \overline{10.10110111111000010}$ 101000101100... while

$\pi = 11.0010 \overline{\mathbf{010000111110110101}} 01000 \dots$

have 19 bits agreeing in base two—with one read right to left

- More extended coincidences are almost always contrived ...
- And strong heuristics exist for believing results like the preceding ζ -function and π examples.
- $\ensuremath{\mathbb{R}}$ But recall the $\ensuremath{\textit{Skewes number}}$

$$\int_2^x \frac{dt}{\log t} \ge \pi(x) \quad \text{failure at } (10^{360})$$

and the *Merten Conjecture*

$$\left|\sum_{k=1}^{n} \mu(k)\right| \leq \sqrt{n}$$
 failure at (10¹¹⁰)

counter-examples.

HIGH PRECISION FRAUD

$$\sum_{n=1}^{\infty} \frac{[n \tanh(\pi)]}{10^n} \stackrel{?}{=} \frac{1}{81}$$

is valid to 268 places; while

$$\sum_{n=1}^{\infty} \frac{\left[n \tanh\left(\frac{\pi}{2}\right)\right]}{10^n} \stackrel{?}{=} \frac{1}{81}$$

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

 $[0, 1, {\color{red}{\bf 267}}, 4, 14, 1, 2, 1, 2, 2, 1, 2, 3, 8, 3, 1]$

and

 $[0, 1, {\color{red}{11}}, 14, 4, 1, 1, 1, 3, 1, 295, 4, 4, 1, 5, 17, 7]$

 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."

DICTIONARIES are LIKE TIMEPIECES

Samuel Johnson observed of watches that "the best do not run true, and the worst are better than none." The same is true of tables and databases. Michael Berry

"would give up Shakespeare in favor of Prudnikov, Brychkov and Marichev."

• That excellent 3 volume compendium contains

$$\sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \frac{1}{k^2 \left(k^2 - kl + l^2\right)} = \frac{\pi^{\alpha} \sqrt{3}}{30}, \quad (4)$$

where the " α " is *probably* "4" [volume 1, entry 9, page 750].

- ★ Integer relation methods suggest that no reasonable value of ∝ works
 - Forensic Mathematics (CSI-Math).
 - what is intended in (4)? There are many such examples (e.g., Lewin on Landen, Fermat's margin)

SIMON and RUSSELL on INDUCTION

This skyhook-skyscraper construction of science from the roof down to the yet unconstructed foundations was possible because the behaviour of the system at each level depended only on a very approximate, simplified, abstracted characterization at the level beneath.¹³

This is lucky, else the safety of bridges and airplanes might depend on the correctness of the "Eightfold Way" of looking at elementary particles.

♦ Herbert A. Simon, The Sciences of the Artificial, MIT Press, 1996, page 16. (An early experimental computational scientist.)

¹³... More than fifty years ago Bertrand Russell made the same point about the architecture of mathematics. See the "Preface" to Principia Mathematica "... the chief reason in favour of any theory on the principles of mathematics must always be inductive, i.e., it must lie in the fact that the theory in question allows us to deduce ordinary *mathematics.* In mathematics, the greatest degree of self-evidence is usually not to be found quite at the beginning, but at some later point; hence the early deductions, until they reach this point, give reason rather for believing the premises because true consequences follow from them, than for believing the consequences because they follow from the premises." Contemporary preferences for deductive formalisms frequently blind us to this important fact, which is no less true today than it was in 1910.

FROM ENIAC: Integrator and Calculator

SIZE/WEIGHT: ENIAC had 18,000 vacuum tubes, 6,000 switches, 10,000 capacitors, 70,000 resistors, 1,500 relays, was 10 feet tall, occupied 1,800 square feet and weighed 30 tons



SPEED/MEMORY: A 1.5GHz Pentium does 3 million adds/sec. ENIAC did 5,000 — 1,000 times faster than any earlier machine. The first stored-memory computer, ENIAC could store 200 digits.

ARCHITECTURE: Data flowed from one accumulator to the next. After each accumulator finished a calculation, it communicated its results to the next in line

The accumulators were connected to each other manually

- The 1949 computation of π to 2,037 places suggested by von Neumann, took 70 hours
- It would have taken roughly 100,000 ENIACs to store the Smithsonian's picture!

⊗ Now after 40 years of Moore's law ...

"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 ... To Moore's Law



The complexity for minimum component costs has increased at a rate of roughly a factor of two per year. ... Over the longer term, the rate of increase is a bit more uncertain, although there is no reason to believe it will not remain nearly constant for at least 10 years.* (Gordon Moore, Intel co-founder, 1965)

*'Expect at least another decade.' (Moore et al)

- An astounding record of sustained exponential progress without peer in history of technology
 - Math tools are now being implemented on parallel platforms, providing *much* greater power to the research mathematician





727-fold speedup of *auadra*ture on the 1K G5's at Virginia **Tech** reduces 3hrs to 15secs

Amassing huge amounts of processing power will not solve many mathematical problems. There are few math 'Grand-challenge problems' — more value in very rapid 'Aha's.

VISUAL DYNAMICS

• In recent continued fraction work, we needed to study the *dynamical system* $t_0 := t_1 := 1$:

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

where $\omega_n = a^2, b^2$ for *n* even, odd respectively. \checkmark Think of this as a **black box**.

▷ Numerically all one *sees* is $t_n \rightarrow 0$ slowly. ▷ Pictorially we *learn* significantly more^{*}:



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

• Scaling by \sqrt{n} , and coloring odd and even iterates, fine structure appears. We now predict and validate:



The attractors for various |a| = |b| = 1
RAMANUJAN'S FRACTION

Chapter 18 of *Ramanujan's Second Notebook* studies the beautiful:

$$\mathcal{R}_{\eta}(a,b) = \frac{a}{\eta + \frac{b^2}{\eta + \frac{4a^2}{\eta + \frac{9b^2}{\eta + \dots}}}}$$
(1.1)

for real, positive $a, b, \eta > 0$. Remarkably, \mathcal{R} satisfies an AGM relation

$$\mathcal{R}_{\eta}\left(\frac{a+b}{2},\sqrt{ab}\right) = \frac{\mathcal{R}_{\eta}(a,b) + \mathcal{R}_{\eta}(b,a)}{2} \qquad (1.2)$$



A scatter plot experiment discovered the domain of convergence for $a/b \in \mathbf{C}$. This is now fully explained with a *lot* of dynamics work.

HADAMARD and GAUSS

The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it.

◊ J. Hadamard quoted at length in E. Borel, Lecons sur la theorie des fonctions, 1928.



Pauca sed Matura

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.*

*Likewise the quote!

De lamaifrate, ellegen liftine omnes expectate ones l'aperantia acquisticimas etgais pre methodos quae campum proofus mun autis aperint. Gott. Int. * Polatio problematis bellister fott that * Cometarum theorian perfect irren redditi Grt Nous inmalysi campus de notis aperuit interet inneftiga tis lanchimmete Th # Formas superiores considerare coop Formulac rouas execting us perially H' Terminum midun arithmotico-geometricum iater 1 at 12 elle = To vigue ad ingüram mileriman compostaciumus quare deminiferata provins nonus rampus in analysi Perminiferata provins nonus rampus in analysi Mr. Maiso 1. certs apericher

Novus in analysi campus se nobis aperuit

An excited young Gauss writes: "A new field of analysis has revealed itself to us, evidently in the study of functions etc." (October 1798)

HALES and KEPLER

- Kepler's conjecture: **the densest way to stack spheres is in a pyramid** is the oldest problem in discrete geometry.
- The most interesting recent example of computer assisted proof. Published in *Annals of Math* with an "only 99% checked" disclaimer.
- This has triggered very varied reactions. (In Math, Computers Don't Lie. Or Do They? NYT 6/4/04)
- Famous earlier examples: the Four Color Theorem and the Non-existence of a Projective Plane of Order 10.
- The three raise and answer quite distinct questions —both real and specious. As does the status of the classification of Finite Simple Groups.
- Formal Proof theory has received an unexpected boost: automated proofs *may* now exist of: Four Color Theorem, Prime Number Theorem.

news feature

Does the proof stack up?

Think peer review takes too long? One mathematician has waited four years to have his paper refereed, only to hear that the exhausted reviewers can't be certain whether his proof is correct. George Szpiro investigates.



Grocers the world over know the most efficient way to stack spheres — but a mathematical proof for the method has brought reviewers to their knees.

ust under five years ago, Thomas Hales made a startling claim. In an e-mail he sent to dozens of mathematicians, Hales declared that he had used a series of computers to prove an idea that has evaded certain confirmation for 400 years. The subject of his message was Kepler's conjecture, proposed by the German astronomer Johannes Kepler, which states that the densest arrangement of spheres is one in which they are stacked in a pyramid — much the same way as grocers arrange oranges.

Soon after Hales made his announcement, reports of the breakthrough appeared on the front pages of newspapers around the world. But today, Hales's proof remains in limbo. It has been submitted to the prestigious *Annals of Mathematics*, but is yet to appear in print. Those charged with checkingit saythat they believe the proof is correct, but are so exhausted with the verification process that they cannot definitively rule out any errors. So when Hales's manuscript finally does appear in the *Annals*, probably during the next year, it will carry an unusual editorial note — a statement that parts of the paper have proved impossible to check.

At the heart of this bizarre tale is the use of computers in mathematics, an issue that has split the field. Sometimes described as a 'brute force' approach, computer-aided proofs often involve calculating thousands of possible outcomes to a problem in order to produce the final solution. Many mathematicians dislike this method, arguing that it is inelegant. Others criticize it for not offering any insight into the problem under consideration. In 1977, for example, a computer-aided proof was published for the four-colour theorem, which states that no more than four colours are needed to fill in a map so that any two adjacent regions have different colours^{1,2}. No errors have been found in the proof, but some mathematicians continue to seek a solution using conventional methods.

Pile-driver

Hales, who started his proof at the University of Michigan in Ann Arbor before moving to the University of Pittsburgh, Pennsylvania, began by reducing the infinite number of possible stacking arrangements to 5,000 contenders. He then used computers to calculate the density of each arrangement. Doing so was more difficult than it sounds. The proof involved checking a series of mathematical inequalities using specially written computer code. In all, more than 100,000 inequalities were verified over a ten-year period.

Robert MacPherson, a mathematician at the Institute for Advanced Study in Princeton, New Jersey, and an editor of the *Annals*, was intrigued when he heard about the proof. He wanted to ask Hales and his graduate student Sam Ferguson, who had assisted with the proof, to submit their finding for publication, but he was also uneasy about the computer-based nature of the work.

The Annalshad, however, already accepted a shorter computer-aided proof — the paper, on a problem in topology, was published this March³. After sounding out his colleagues on the journal's editorial board, MacPherson asked Hales to submit his paper. Unusually, MacPherson assigned a dozen mathematicians to referee the proof — most journals tend to employ between one and three. The effort was led by Gábor Fejes Tóth of the Alfréd Rényi Institute of Mathematics in Budapest, Hungary, whose father, the mathematician László Fejes Tóth, had predicted in 1965 that computers would one day make a proof of Kepler's conjecture possible.

It was not enough for the referees to rerun Hales's code — they had to check whether the programs did the job that they were supposed to do. Inspecting all of the code and its inputs and outputs, which together take up three gigabytes of memory space, would have been impossible. So the referees limited themselves to consistency checks, a reconstruction of the thought processes behind each step of the proof, and then a

news feature

S. TERRY/SPI

study of all of the assumptions and logic used to design the code. A series of seminars, which ran for full academic years, was organized to aid the effort.

But success remained elusive. Last July, Fejes Tóth reported that he and the other referees were 99% certain that the proof is sound. They found no errors or omissions, but felt that without checking every line of the code, they could not be absolutely certain that the proof is correct.

For a mathematical proof, this was not enough. After all, most mathematicians believe in the conjecture already — the proof is supposed to turn that belief into certainty. The history of Kepler's conjecture also gives reason for caution. In 1993, Wu-Yi Hsiang, then at the University of California, Berkeley, published a 100-page proof of the conjecture in the *International Journal of Mathematics*⁴. But shortly after publication, errors were found in parts of the proof. Although Hsiang stands by his paper, most mathematicians do not believe it is valid.

After the referees' reports had been considered, Hales says that he received the following letter from MacPherson: "The news from the referees is bad, from my perspective. They have not been able to certify the correctness of the proof, and will not be able to certify it in the future, because they have run out of energy ... One can speculate whether their process would have converged to a definitive answer had they had a more clear manuscript from the beginning, but this does not matter now."

NATURE VOL 424 3 JULY 2003 www.nature.com/nature

Pyramid power:

Thomas Hales

believes that

succeed where

computers will

humans have failed

in verifying

his proof.

JNIV. PITTSBURGH CIDDE



Star player: Johannes Kepler's conjecture has kept mathematicians guessing for 400 years.

The last sentence lets some irritation shine through. The proof that Hales delivered was by no means a polished piece. The 250-page manuscript consisted of five separate papers, each a sort of lab report that Hales and Ferguson filled out whenever the computer finished part of the proof. This unusual format made for difficult reading. To make matters worse, the notation and definitions also varied slightly between the papers.

Rough but ready

MacPherson had asked the authors to edit their manuscript. But Hales and Ferguson did not want to spend another year reworking their paper. "Tom could spend the rest of his career simplifying the proof," Ferguson said when they completed their paper. "That doesn't seem like an appropriate use of his time." Hales turned to other challenges, using traditional methods to solve the 2,000-year-old honeycomb conjecture, which states that of all conceivable tiles of equal area that can be used to cover a floor without leaving any gaps, hexagonal tiles have the shortest perimeter⁵. Ferguson left academia to take a job with the US Department of Defense.

Faced with exhausted referees, the editorial board of the *Annals* decided to publish the paper — but with a cautionary note. The paper will appear with an introduction by the editors stating that proofs of this type, which involve the use of computers to check a large number of mathematical statements, may be impossible to review in full. The matter might have ended there, but for Hales, having a note attached to his proof was not satisfactory.

This January, he launched the Flyspeck project, also known as the Formal Proof of Kepler. Rather than rely on human referees, Hales intends to use computers to verify every step of his proof. The effort will require the collaboration of a core group of about ten volunteers, who will need to be qualified mathematicians and willing to donate the computer time on their machines. The team will write programs to deconstruct each step of the proof, line by line, into a set of axioms that are known to be correct. If every part of the code can be broken down into these axioms, the proof will finally be verified.

Those involved see the project as doing more than just validating Hales's proof. Sean McLaughlin, a graduate student at New York University, who studied under Hales and has used computer methods to solve other mathematical problems, has already volunteered. "It seems that checking computerassisted proofs is almost impossible for humans," he says. "With luck, we will be able to show that problems of this size can be subjected to rigorous verification without the need for a referee process."

But not everyone shares McLaughlin's enthusiasm. Pierre Deligne, an algebraic geometer at the Institute for Advanced Study, is one of the many mathematicians who do not approve of computer-aided proofs. "Ibelieve in a proof if I understand it,"he says. For those who side with Deligne, using computers to remove human reviewers from the refereeing process is another step in the wrong direction.

Despite his reservations about the proof, MacPherson does not believe that mathematicians should cut themselves off from computers. Others go further. Freek Wiedijk, of the Catholic University of Nijmegen in the Netherlands, is a pioneer of the use of computers to verify proofs. He thinks that the process could become standard practice in mathematics. "People will look back at the turn of the twentieth century and say that is when it happened,"Wiedijk says.

Whether or not computer-checking takes off, it is likely to be several years before Flyspeck produces a result. Hales and McLaughlin are the only confirmed participants, although others have expressed an interest. Hales estimates that the whole process, from crafting the code to running it, is likely to take 20 person-years of work. Only then will Kepler's conjecture become Kepler's theorem, and we will know for sure whether we have been stacking oranges correctly all these years.

George Szpiro writes for the Swiss newspapers NZZ and NZZ am Sonntag from Jerusalem, Israel. His book Kepler's Conjecture (Wiley, New York) was published in February.

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Flyspeck

www.math.pitt.edu/~thales/flyspeck/index.html

13

Mathematics

What in the Name of Euclid Is Going On Here?

Computer assistants may help mathematicians dot the i's and cross the t's of proofs so complex that they defy human comprehension

In 1998, a young University of Michigan mathematician named Thomas Hales solved a nearly 4-century-old problem called the Kepler conjecture. The task was to prove that the standard grocery-store arrangement of oranges is, in fact, the densest way to pack spheres together. The editor of *Annals of Mathematics*, one of the most prestigious journals in mathematics, invited him to submit his proof to *Annals*. Neither of them was prepared for what happened next.

Over a period of 4 years, a team of 12 referees wrestled with the lengthy paper and eventually raised a white flag. They informed the editor that they were only "99 percent" certain that it was correct. In particular, they could not vouch for the validity of the lengthy computer calculations that were essential to Hales's proof. The editor took the unprecedented step of publishing the article with a disclaimer that it could not be absolutely verified (*Science*, 7 March 2003, p. 1513).

It is a scenario that has repeated itself, with variations, several times in recent years: A high-profile problem is solved with an extraordinarily long and difficult megaproof, sometimes relying heavily on computer calculation and often leaving a miasma of doubt behind it. In 1976, the Four Color Theorem started the trend, with a proof based on computer calculations so lengthy that no human could hope to follow them. The classification of finite simple groups, a 10,000-page multiauthor project, was completed (sort of) in 1980 but had to be recompleted last year. "We've arrived at a strange place in mathematics," says David Goldschmidt of the Institute for Defense Analyses in Alexandria, Virginia, one of the collaborators on the finite simple group proof. "When is a proof really a proof? There's no absolute standard." Goldschmidt thinks the traditional criterionreview by a referee (or team of them)breaks down when a paper reaches hundreds or thousands of pages.

The computer—which at first sight seems to be part of the problem—may also be the solution. In the past few months, software packages called "proof assistants," which go through every step of a carefully written argument and check that it follows from the axioms of mathematics, have served notice that they are no longer toys. Last fall, Jeremy Avigad, a professor of philosophy at Carnegie



Mapping the way. Georges Gonthier's computer verified billions of calculations on "hypermaps" like the one shown.

Mellon University, used a computer assistant called Isabelle to verify the Prime Number Theorem, which (roughly speaking) describes the probability that a randomly chosen number in any interval is prime. And in December, Georges Gonthier, a computer scientist at Microsoft Research Cambridge, announced a successful verification of the proof of the Four Color Theorem, using a proof assistant called Coq. "It's finally getting to the stage where you can do serious things with these programs," says Avigad.

Even Hales is getting into the action. Over the past 2 years, he has taught himself to use an assistant called HOL Light. In January, he became the first person to complete a computer verification of the Jordan Curve Theorem, first published in 1905, which says that any closed curve drawn in the plane without crossing itself separates the plane into two pieces.

For Hales, the motivation is obvious: He hopes, eventually, to vindicate his proof of the Kepler conjecture. In fact, three graduate students in Europe (not Hales's own) are already

at work on separate parts of this project, two using Isabelle and one using Coq. Hales expects them to finish in about 7 years.

But Hales thinks that computer verifiers have implications far beyond the Kepler conjecture. "Suppose you could check a page a day," he says. "At that point it would make sense to devote the resources to put 100,000 pages of mathematics into one of these systems. Then the mathematical landscape is entirely changed." At present, computer assistants still take a lot of time to puzzle through some facts that even an advanced undergraduate would know or be able to figure out. With a large enough knowl-

edge base, that particular time sink could be eliminated, and the programs might enable mathematicians to work more efficiently. "My own experience is that you spend a long time going over and going over a proof, making sure you haven't missed anything," says Carlos Simpson, an algebraic geometer and computer scientist at the University of Nice in France. "With the computer, once it's proved, it's proved. You only have to do it once, and the computer makes sure you get all the details."

In fact, computer proof assistants could change the whole concept of proof. Ever since Euclid, mathematical proofs have served a dual purpose: certifying *that* a statement is true, and explaining *why* it is

Have a Coq and a Smile

Why would hundreds of computer scientists devote more than 30 years to developing mathematical proof assistants that most mathematicians don't even want? The answer is that they are chasing an even more elusive grail: self-checking computer code.

In a sense, the statement "this program (or chip, or operating system) performs task x correctly" is a mathematical theorem, and programmers would love to have that kind of certainty. "Currently, people who have experience with programming 'know' that serious programs without bugs are impossible," Freek Wiedijk and Henk Barendregt, computer scientists at the University of Nijmegen in the Netherlands, wrote in 2003. "However, we think that eventually the technology of computer mathematics... will change this perception."

Already, leading chip manufacturers use computer proof assistants to make sure their circuit designs are correct. Advanced Micro Devices uses a proof checker called ACL2, and Intel uses HOL Light. "When the division algorithm turned out to be wrong on the Pentium chip, that was a real wake-up call to Intel," says John Harrison, who designed HOL Light and was subsequently hired as a senior software engineer by Intel. –D.M.

MORE of OUR 'METHODOLOGY'

- 1. (*High Precision*) computation of object(s)
- Pattern Recognition of Real Numbers (The Inverse Symbolic Calculator* and 'identify' or 'Recognize')

 $identify(\sqrt{2.} + \sqrt{3.}) = \sqrt{2} + \sqrt{3}$

- 3. *Pattern Recognition of Sequences* (Salvy & Zimmermann's 'gfun', Sloane & Plouffe's *Encyclopedia*).
- 4. Much use of 'Integer Relation Methods':[†]
 - ✓ "Exclusion bounds" are especially useful
 - ✓ Great test bed for "Experimental Math"
- 5. Some automated theorem proving (Wilf-Zeilberger etc)

 *ISC space limits: from 10Mb in 1985 to 10Gb today.
 [†]PSLQ, LLL, FFT. Top Ten "Algorithm's for the Ages," Random Samples, Science, Feb. 4, 2000.

Another Truth

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt \stackrel{?}{=} L_{-7}(2) \quad (5)$$

where

$$L_{-7}(s) = \sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^s} + \frac{1}{(7n+2)^s} - \frac{1}{(7n+3)^s} + \frac{1}{(7n+4)^s} - \frac{1}{(7n+5)^s} - \frac{1}{(7n+6)^s} \right]$$

- Equation (5) arises from volumes of ideal tetrahedron in hyperbolic space. For algebraic topology reasons, it is known that the ratio of lefthand to right-hand side of (5) is rational.
- "Identity" (5) has been verified to 20,000 places.
 I have *no idea* of how to prove it.
- A 64-CPU 10,000 digit run (7250 secs) and a 256-CPU run (1855 secs) on the Virginia Tech G5 cluster agreed precisely—a week in an hour: 20,000 in 3104 secs on 1024-CPUs and 900 fold speed up: the largest numerical quadrature calculation ever done?

JOHN MILNOR

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





ZEROES of 0 – 1 POLYNOMIALS



Data mining in polynomials

• The striations are unexplained!

WHAT YOU DRAW is WHAT YOU SEE



The price of metaphor is eternal vigilance

(Arturo Rosenblueth & Norbert Wiener)

SEEING PATTERNS in PARTITIONS

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

$$1 + \sum_{n \ge 1} p(n)q^n = \frac{1}{\prod_{n \ge 1} (1 - q^n)}.$$
 (6)

Thus, p(5) = 7 since

$$5 = 4 + 1 = 3 + 2 = 3 + 1 + 1 = 2 + 2 + 1$$

= 2 + 1 + 1 + 1 = 1 + 1 + 1 + 1 + 1.

- Developing (6) is an introduction to enumeration via *generating functions* as discussed in Polya's change example.
- Additive partitions are harder to handle than multiplicative factorizations, but they may be introduced in the elementary school curriculum with questions like:

How many 'trains' of a given length can be built with Cuisenaire rods? Ramanujan used MacMahon's 1900 table for p(n) to intuit remarkable deep congruences like

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

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

from relatively limited data like P(q) =

$$1 + q + 2q^{2} + 3q^{3} + 5q^{4} + 7q^{5} + 11q^{6} + 15q^{7} + 22q^{8} + 30q^{9} + 42q^{10} + 56q^{11} + 77q^{12} + 101q^{13} + 135q^{14} + 176q^{15} + 231q^{16} + 297q^{17} + 385q^{18} + 490q^{19} + 627q^{20} + 792q^{21} + 1002q^{22} + 1255q^{23} + 1575q^{24} + \dots + 3972999029388q^{200} + \dots$$
(7)

- Cases 5n + 4 and 7n + 5 are flagged in (7)
 - leading to the *crank* (Dyson, Andrews, Garvan, Ono, and very recently Mahlburg)
 - connections with modular forms much facilitated by symbolic computation
- Of course, it is easier to (heuristically) confirm than find these fine examples of Mathematics: the science of patterns.*

*Keith Devlin's 1997 book.

IS HARD or EASY BETTER?

A modern computationally driven question is How hard is p(n) to compute?

- In **1900**, it took the father of combinatorics, Major Percy MacMahon (1854–1929), months to compute p(200) using recursions developed from (6).
- By 2000, Maple produced p(200) in seconds simply as the 200'th term of the Taylor series (ignoring 'combinat[numpart]')
- A few years earlier it required being careful to compute the series for $\prod_{n\geq 1}(1-q^n)$ first and then the series for the reciprocal of that series!
- This baroque event is occasioned by *Euler's pen*tagonal number theorem

$$\prod_{n\geq 1} (1-q^n) = \sum_{n=-\infty}^{\infty} (-1)^n q^{(3n+1)n/2}.$$

 The reason is that, if one takes the series for (6), the software has to deal with 200 terms on the bottom.

But the series for $\prod_{n\geq 1}(1-q^n)$, has only to handle the **23** non-zero terms in series in the pentagonal number theorem.

• If introspection fails, we can find and learn about the *pentagonal numbers* occurring above in Neil *Sloanes'* exemplary on-line

'Encyclopedia of Integer Sequences':

www.research.att.com/personal/njas/sequences/eisonline.html

Such ex post facto algorithmic analysis can be used to facilitate independent student discovery of the pentagonal number theorem, and like results.

- The difficulty of estimating the size of p(n) analytically —so as to avoid enormous or unattainable computational effort—led to some marvellous mathematical advances*.
- The corresponding ease of computation may now act as a retardant to insight.
- ★ New mathematics is often discovered only when prevailing tools run totally out of steam.
 - This raises a caveat against mindless computing:

Will a student or researcher discover structure when it is easy to compute without needing to think about it? Today, she may thoughtlessly compute p(500)which a generation ago took much, much pain and insight.

*By researchers including Hardy and Ramanujan, and Rademacher

BERLINSKI

The body of mathematics to which the calculus gives rise embodies a certain swashbuckling style of thinking, at once bold and dramatic, given over to large intellectual gestures and indifferent, in large measure, to any very detailed description of the world.

It is a style that has shaped the physical but not the biological sciences, and its success in Newtonian mechanics, general relativity and quantum mechanics is among the miracles of mankind. But the era in thought that the calculus made possible is coming to an end. Everyone feels this is so and everyone is right. The computer has in turn changed the very nature of mathematical experience, suggesting for the first time that mathematics, like physics, may yet become an empirical discipline, a place where things are discovered because they are seen. (David Berlinski, 1997)*

- As all sciences rely more on 'dry experiments', via computer simulation, the boundary between physics (e.g., *string theory*) and mathematics (e.g., *by experiment*) is again delightfully blurred.
- An early exciting example is provided by gravitational boosting:

*In "Ground Zero", a Review of *The Pleasures of Counting*, by T. W. Koerner.

MATH AWARENESS MONTH

• *Interactive graphics* will become an integral part of mathematics: gravitational boosting, gravity waves, Lagrange points, many-body problems



1905 Special relativity, Brownian motion, Photoelectricity

Gravitational Boosting

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

The article starts by quoting Arthur C. Clarke

"Any sufficiently advanced technology is indistinguishable from magic."



Sedna and Friends in 2004

Until he showed *Hohmann transfer ellipses* were not least energy paths to the outer planets:

"most planetary mission designers considered the gravity field of a target planet to be somewhat of a nuisance, to be cancelled out, usually by onboard Rocket thrust."



- Without a boost from the orbits of Saturn, Jupiter and Uranus, the Earth-to-Neptune Voyager mission (achieved in 1989 in around a decade) would have taken over 30 years!
- We would still be waiting; longer to see Sedna confirmed (8 billion miles away—3 times further than Pluto).

LIGO: Math and the Cosmos

Einstein's theory of general relativity describes how massive bodies curve space and time; it realizes gravity as movement of masses along shortest paths in curved space-time.

• A subtle mathematical inference is that relatively accelerating bodies will produce ripples on the curved space-time surface, propagating at the speed of light: *gravitational waves*.

These extraordinarily weak cosmic signals hold the key to a new era of astronomy *if only* we can build detectors and untangle the mathematics to interpret them. The signal to noise ratio is tiny! **LIGO**, the Laser Interferometer Gravitational-Wave Observatory, is such a developing US gravitational wave detector.



One of the first 3D simulations of the gravitational waves arising when two black holes collide

 Only recently has the computational power existed to realise such simulations, on computers such as at WestGrid (www.westgrid.ca)

SOME CONCLUSIONS

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. (Thomas Kuhn)

• In Who Got Einstein's Office? (Beurling)

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." (Einstein)

HILBERT

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.

Besides it is an error to believe that rigor in the proof is the enemy of simplicity. (David Hilbert, 1900)

. . .

 In his '23' "Mathematische Probleme" lecture to the Paris International Congress, 1900*

*See Ben Yandell's fine account in *The Honors Class*, AK Peters, 2002.

CHAITIN

I believe that elementary number theory and the rest of mathematics should be pursued more in the spirit of experimental science. and that you should be willing to adopt new principles. I believe that Euclid's statement that an axiom is a self-evident truth is a big mistake^{*}. The Schrödinger equation certainly isn't a self-evident truth! And the Riemann Hypothesis isn't self-evident either, but it's very useful. A physicist would say that there is ample experimental evidence for the Riemann Hypothesis and would go ahead and take it as a working assumption.

^{*}There is no evidence that Euclid ever made such a statement. However, the statement does have an undeniable emotional appeal.

In this case, we have ample experimental evidence for the truth of our identity and we may want to take it as something more than just a working assumption. We may want to introduce it formally into our mathematical system. (Greg Chaitin, 1994)*



A tangible **Riemann surface for Lambert-***W*

*A like article is in the 2004 Mathematical Intelligencer.

FINAL COMMENTS

- ★ The traditional deductive accounting of Mathematics is a largely ahistorical caricature*
- ★ Mathematics is primarily about secure knowledge not proof, and the aesthetic is central
 - Proofs are often out of reach understanding, even certainty, is not
 - Packages can make concepts accessible (Linear relations, Galois theory, Groebner bases)
 - While progress is made "one funeral at a time" (Niels Bohr), "you can't go home again" (Thomas Wolfe).

*Quotations are at jborwein/quotations.html

HOW NOT TO EXPERIMENT

mc² Einstein \$ +2mo(E-V(r))\$ = 0 Jehrödinger &fa)dz=0 Caochy-Gousat NEWLE BETT

Pooh Math

'Guess and Check' while Aiming Too High

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APPENDIX I. ANOTHER CASE STUDY

LOG-CONCAVITY

Consider the *unsolved* **Problem 10738** in the 1999 *American Mathematical Monthly*:

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^{*} 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 $t \ge 1$.

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

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 $2jk \le k^2 + j^2$.

(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

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

In particular for t = 1, we obtain the sequence

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

- These are the *Bell numbers* as was discovered by consulting *Sloane's Encyclopedia*.
 www.research.att.com/personal/njas/sequences/index.html
- Sloane can also tell us that, for t = 2, we have the generalized Bell numbers, and gives the exponential generating functions.*

▶ Inter alia, an explicit computation shows that

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

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

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

$$\sum_{n \ge 0} c_n u^n = \exp\left(t(e^u - 1)\right).$$
 (8)

*The Bell numbers were known earlier to Ramanujan — an example of *Stigler's Law of Eponymy*!

 $(c^*)^*$ We appeal to a recent theorem due to E. Rodney Canfield,[†] which proves the lovely and quite difficult result below.

Theorem 1 If a sequence $1, b_1, b_2, \cdots$ is non-negative 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 (8) above, we apply this to the sequence $\mathbf{b_j} = \mathbf{t}/(\mathbf{j} - 1)!$ which is log-concave exactly for $t \ge 1$. QED

The '' indicates this was the unsolved component.

[†]A search in 2001 on *MathSciNet* for "Bell numbers" since 1995 turned up 18 items. This paper showed up as number 10. Later, *Google* found it immediately!
• It transpired that the given solution to (c) was the only one received by the *Monthly*

► This is quite unusual

• The reason might well be that it relied on the following sequence of steps:

(??) \Rightarrow Computer Algebra System \Rightarrow Interface

 \Rightarrow Search Engine \Rightarrow Digital Library

 \Rightarrow Hard New Paper \Rightarrow **Answer**

 \star Now if only we could automate this!

Experimental Mathematics:

2×Ten Computational Challenge Problems

Jonathan M. Borwein, FRSC

Research Chair in IT Dalhousie University

Halifax, Nova Scotia, Canada

2005 Clifford Lecture III

Tulane, March 31–April 2, 2005

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. ... Besides it is an error to believe that rigor in the proof is the enemy of simplicity. (David Hilbert, 1900)



AK Peters 2004

DALHOUSIE UNIVERSITY

Inspiring Minds

Talk Revised: 03–20–05

This lecture will make a more advanced analysis of the themes developed in Lectures 1 and 2. It will look at 'lists and challenges' and discuss two sets of *Ten Computational Mathematics Problems* including

$$\int_0^\infty \cos(2x) \prod_{n=1}^\infty \cos\left(\frac{x}{n}\right) \, dx \stackrel{?}{=} \frac{\pi}{8}.$$

This problem set was stimulated by Nick Trefethen's recent more numerical *SIAM 100 Digit*, *100 Dollar Challenge*.*

 We start with a general description of the Digit Challenge[†] and finish with an examination of some of its components.

*The talk is based on an article to appear in the May 2005 *Notices of the AMS*, and related resources such as www.cs.dal.ca/~jborwein/digits.pdf.

[†]Quite full details of which are beautifully recorded on Bornemann's website www-m8.ma.tum.de/m3/bornemann/challengebook/ which accompanies *The Challenge*.



Lists, Challenges, and Competitions

These have a long and primarily lustrous—social constructivist—history in mathematics.

- Consider the Hilbert Problems*, the Clay Institute's seven (million dollar) Millennium problems, or Dongarra and Sullivan's 'Top Ten Algorithms'.
- We turn to the story of a recent highly successful challenge.

The book under review also makes it clear that with the continued advance of computing power and accessibility, the view that "real mathematicians don't compute" has little traction, especially for a newer generation of mathematicians who may readily take advantage of the maturation of computational packages such as Maple, Mathematica and MATLAB. (JMB, 2005)

*See the late Ben Yandell's wonderful *The Honors Class: Hilbert's Problems and Their Solvers*, A K Peters, 2001.

Numerical Analysis Then and Now

Emphasizing quite how great an advance positional notation was, Ifrah writes:

A wealthy (15th Century) German merchant, seeking to provide his son with a good business education, consulted a learned man as to which European institution offered the best training. "If you only want him to be able to cope with addition and subtraction," the expert replied, "then any French or German university will do. But if you are intent on your son going on to multiplication and division – assuming that he has sufficient gifts – then you will have to send him to Italy. (Georges Ifrah*)

*From page 577 of *The Universal History of Numbers: From Prehistory to the Invention of the Computer*, translated from French, John Wiley, 2000.

Archimedes method

George Phillips has accurately called Archimedes the first numerical analyst. In the process of obtaining his famous estimate

$$3 + \frac{10}{71} < \pi < 3 + \frac{10}{70}$$

he had to master notions of recursion without computers, interval analysis without zero or positional arithmetic, and trigonometry without any of our modern analytic scaffolding ...

A modern computer algebra system can tell one that

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

since the integral may be interpreted as the area under a positive curve.

We are though no wiser as to why! If, however, we ask the same system to compute the indefinite integral, we are likely to be told that

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

Now (1) is rigourously established by differentiation and an appeal to the Fundamental theorem of calculus. $\hfill \Box$



Archimedes' method for π with 6- and 12-gons



A random walk on one million digits of $\boldsymbol{\pi}$

- While there were many fine arithmeticians over the next 1500 years, Ifrah's anecdote above shows how little had changed, other than to get worse, before the Renaissance.
- By the 19th Century, Archimedes had finally been outstripped both as a theorist, and as an (applied) numerical analyst:

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

*Quoted by Adrian Rice in "What Makes a Great Mathematics Teacher?" on page 542 of The American Mathematical Monthly, June-July 1999.



Archimedes: 223/71 < π < 22/7

A pictorial proof

- De Morgan seems to have been one of the first to mistrust William Shanks's epic computations of Pi—to 527, 607 and 727 places, noting there were too few sevens.
- But the error was only confirmed three quarters of a century later in 1944 by Ferguson with the help of a calculator in the last pre-computer calculations of π .*
- Until around 1950 a "computer" was still a person and ENIAC was an "Electronic Numerical Integrator and Calculator" on which Metropolis and Reitwiesner computed Pi to 2037 places in 1948 and confirmed that there were the expected number of sevens.
- *A Guinness record for finding an error in math literature?

Reitwiesner, then working at the Ballistics Research Laboratory, Aberdeen Proving Ground in Maryland, starts his article with:

Early in June, 1949, Professor John von Neumann expressed an interest in the possibility that the ENIAC might sometime be employed to determine the value of π and e to many decimal places with a view to toward obtaining a statistical measure of the randomness of distribution of the digits.

The paper notes that *e*appears to be *too random* this is now proven—and ends by respecting an oftneglected 'best-practice':

Values of the auxiliary numbers arccot 5 and arccot 239 to 2035D ... have been deposited in the library of Brown University and the UMT file of MTAC.

 Just as layers of software, hardware & middleware have stabilized, so have their roles in scientific and especially mathematical computing.

- Thirty years ago, LP texts concentrated on 'Y2K'like tricks for limiting storage demands.
 - Now serious users and researchers will often happily run large-scale problems in MATLAB and other broad spectrum packages, or rely on NAG library routines.
 - While such out-sourcing or commoditization of scientific computation and numerical analysis is not without its drawbacks, the analogy with automobile driving in 1905 and 2005 is apt.
- We are now in possession of mature—not to be confused with 'error-free'—technologies. We can be fairly comfortable that *Mathematica* is sensibly handling round-off or cancelation error, using reasonable termination criteria etc.
 - Below the hood, *Maple* is optimizing polynomial computations using tools like Horner's rule, running multiple algorithms when there is no clear best choice, and switching to reduced complexity (Karatsuba or FFT-based) multiplication when accuracy so demands.*

*Though, it would be nice if all vendors allowed as much peering under the bonnet as *Maple* does.

About the Contest

In a 1992 essay "*The Definition of Numerical Analysis*"*. Trefethen engagingly demolishes the conventional definition of Numerical Analysis as "*the science of rounding errors*". He explores how this hyperbolic view emerged and finishes by writing:

I believe that the existence of finite algorithms for certain problems, together with other historical forces, has distracted us for decades from a balanced view of numerical analysis. ... For guidance to the future we should study not Gaussian elimination and its beguiling stability properties, but the diabolically fast conjugate gradient iteration, or Greengard and Rokhlin's O(N) multipole algorithm for particle simulations, or the exponential convergence of spectral methods for solving certain PDEs, or the convergence in O(N) iteration achieved by multigrid methods for many kinds of problems, or even Borwein and Borwein's magical AGM iteration for determining 1,000,000 digits of π in the blink of an eye. That is the heart of numerical analysis.

*SIAM News, November 1992.

In *SIAM News* (Jan 2002), Trefethen liste ten diverse problems used in teaching *modern* graduate numerical analysis in Oxford. Readers were challenged to compute 10 digits of each, with a dollar per digit (\$100) prize to the best entry. Trefethen wrote,

"If anyone gets 50 digits in total, I will be impressed."

- And he was, 94 teams from 25 nations submitted results. Twenty of these teams received a full 100 points (10 correct digits for each problem).
 - They included the late John Boersma working with Fred Simons and others, Gaston Gonnet (a *Maple* founder) and Robert Israel, a team containing Carl Devore, and the current authors variously working alone and with others.
 - An originally anonymous donor, William J. Browning, provided funds for a \$100 award to each of the twenty perfect teams.
 - JMB, David Bailey* and Greg Fee entered, but failed to qualify for an award.[†]

*Bailey wrote the introduction to the book under review. [†]We took Nick at his word and turned in 85 digits!

The Ten Digit Challenge Problems

The purpose of computing is insight, not numbers.* (Richard Hamming)

- #1. What is $\lim_{\epsilon \to 0} \int_{\epsilon}^{1} x^{-1} \cos(x^{-1} \log x) dx$?
- #2. A photon moving at speed 1 in the x-y plane starts at t = 0 at (x, y) = (1/2, 1/10) heading due east. Around every integer lattice point (i, j) in the plane, a circular mirror of radius 1/3 has been erected. How far from the origin is the photon at t = 10?
- #3. The infinite matrix A with entries $a_{11} = 1$, $a_{12} = 1/2$, $a_{21} = 1/3$, $a_{13} = 1/4$, $a_{22} = 1/5$, $a_{31} = 1/6$, etc., is a bounded operator on ℓ^2 . What is ||A||?

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

*In Numerical Methods for Scientists and Engineers, 1962.

- #5. Let $f(z) = 1/\Gamma(z)$, where $\Gamma(z)$ is the gamma function, and let p(z) be the cubic polynomial that best approximates f(z) on the unit disk in the supremum norm $|| \cdot ||_{\infty}$. What is $||f p||_{\infty}$?
- #6. A flea starts at (0,0) on the infinite 2-D integer lattice and executes a biased random walk: At each step it hops north or south with probability 1/4, east with probability $1/4 + \epsilon$, and west with probability $1/4 - \epsilon$. The probability that the flea returns to (0,0) sometime during its wanderings is 1/2. What is ϵ ?
- #7. Let A be the 20000 × 20000 matrix whose entries are zero everywhere except for the primes 2,3,5,7,...,224737 along the main diagonal and the number 1 in all the positions a_{ij} with |i-j| = 1,2,4,8,...,16384. What is the (1,1) entry of A^{-1} .

- #8. A square plate $[-1,1] \times [-1,1]$ is at temperature u = 0. At time t = 0 the temperature is increased to u = 5 along one of the four sides while being held at u = 0 along the other three sides, and heat then flows into the plate according to $u_t = \Delta u$. When does the temperature reach u = 1 at the center of the plate?
- #9. The integral $I(\alpha) = \int_0^2 [2 + \sin(10\alpha)] x^{\alpha} \sin(\alpha/(2 x)) dx$ depends on the parameter α . What is the value $\alpha \in [0, 5]$ at which $I(\alpha)$ achieves its maximum?
- #10. A particle at the center of a 10×1 rectangle undergoes Brownian motion (i.e., 2-D random walk with infinitesimal step lengths) till it hits the boundary. What is the probability that it hits at one of the ends rather than at one of the sides?

Answers correct to 40 digits are at

web.comlab.ox.ac.uk/oucl/work/nick.trefethen/hundred.html

About the Book and Its Authors

Success in solving these problems requires a broad knowledge of mathematics and numerical analysis, together with significant computational effort, to obtain solutions and ensure correctness of the results.

- The strengths and limitations of Maple, Mathematica, Matlab (The 3Ms), and other software tools such as PARI or GAP, are strikingly revealed in these ventures.
- Almost all of the solvers relied in large part on one or more of these three packages, and while most solvers attempted to confirm their results, there was no explicit requirement for proofs to be provided.
- In December 2002, Keller wrote:

To the Editor: ... found it surprising that no proof of the correctness of the answers was given. Omitting such proofs is the accepted procedure in scientific computing. However, in a contest for calculating precise digits, one might have hoped for more.

Joseph B. Keller, Stanford University

Keller's request for proofs as opposed to compelling evidence of correctness is, in this context, somewhat unreasonable and even in the long-term somewhat counter-productive.

Nonetheless, the *The Challenge* makes a complete and cogent response to Keller and much much more. The interest in the contest has extended to *The Challenge*, which has already received reviews in places such as *Science* where mathematics is not often seen.

- Different readers, depending on temperament, tools and training will find the same problem more or less interesting and more or less challenging.
- Problems can be read independently: multiple solution techniques are given, background, implementation details—variously in each of the *3Ms* or otherwise—and extensions are discussed.
- Each problem has its own chapter and lead author: Folkmar Bornemann, Dirk Laurie, Stan Wagon and Jörg Waldvogel come from 4 countries on 3 continents and did not know each other, though Dirk did visit Jörge and Stan visited Folkmar as they were finishing up.

Some High Spots

The book proves the growing power of collaboration, networking and the grid—both human and computational. A careful reading *yields proofs of correctness for all problems except* for #1, #3 and #5.

- For **#5** one difficulty is to develop a *robust interval implementation* for both complex computation and, more importantly, for the *Gamma function*. Error bounds for **#1** may be out of reach, but an analytic solution to **#3** seems tantalizingly close.
- The authors ultimately provided **10,000-digit solutions** to **nine** of the problems. They say that this improved their knowledge on several fronts as well as being 'cool'.
 - success with Integer Relation Methods often demands ultrahigh precision computation.
- One (and only one) problem remains totally intractable —by this rarefied measure. As of today only 300 digits of #3 are known.

Some Surprising Outcomes

The authors^{*} were surprised by the following:

- #1. The best algorithm for 10,000 digits was the trusty trapezoidal rule—a not uncommon personal experience of mine.
- #2. Using *interval arithmetic* with starting intervals of size smaller than 10^{-5000} , one can still find the position of the particle at time 2000 (not just time ten), which makes a fine exercise for very high-precision interval computation.
- #4. Interval analysis algorithms can handle similar problems in higher dimensions. As a foretaste of future graphic tools, one can solve this problem using current adaptive 3-D plotting routines which can catch all the bumps.

As an optimizer by background this was the first problem my group solved using a damped Newton method.

*Stan Wagon and Folkmar Bornemann, private communications.

- #5. While almost all canned optimization algorithms failed, *differential evolution*, a relatively new type of evolutionary algorithm worked quite well.
- #6 This has an almost-closed form via *elliptic integrals* and leads to a study of random walks on hypercubic lattices, and *Watson integrals*
- #9. The maximum parameter is expressible in terms of a *MeijerG function*. Unlike most contestants, *Mathematica* and *Maple* both figure this out.
 - This is another measure of the changing environment.* It is a good idea—and not at all immoral—to data-mine and find out what your one of the 3Ms knows about your current object of interest. Thus, Maple says:

The Meijer G function is defined by the inverse Laplace transform

*As is Lambert W, see Brian Hayes' Why W?

Two Big Surprises

Two solutions really surprised the authors: #7 Too Large to be Easy, Too Small to Be Hard.

Not so long ago a $20,000 \times 20,000$ matrix was large enough to be hard. Using both *congruential* and *padic methods*, Dumas, Turner and Wan obtained a fully *symbolic* answer, a rational with a 97,000-digit numerator and like denominator. Wan has reduced the time needed to 15 minutes on one machine, from using many days on many machines.

- While p-adic analysis is parallelizable it is less easy than with congruential methods; *the need for better parallel algorithms lurks below the surface* of much modern computational math.
- The surprise here, though, is not that the solution is rational, but that it can be explicitly constructed.

The chapter, like the others offers an interesting menu of numeric and exact solution strategies. Of course, in any numeric approach *illconditioning* rears its ugly head while the use of *sparsity* and other core topics come into play.

Problem #10: Hitting the Ends

(My personal favourite, for reasons that may be apparent.) Bornemann starts the chapter by exploring *Monte-Carlo methods*, which are shown to be impracticable.

- He then reformulates the problem *deterministically* as the value at the center of a 10 × 1 rectangle of an appropriate harmonic measure of the ends, arising from a 5-point discretization of *Laplace's equation* with Dirichlet boundary conditions.
- This is then solved by a well chosen *sparse Cholesky* solver. At this point a reliable numerical value of

$$3.837587979 \cdot 10^{-7}$$

is obtained.

And the posed problem is solved numerically to the requisite 10 places.

But this is only the warm up ...

Analytic Solutions

We proceed to develop two analytic solutions, the first using *separation of variables*^{*} on the underlying PDE on a general $2a \times 2b$ rectangle. We learn that

$$p(a,b) = \frac{4}{\pi} \sum_{k=0}^{\infty} \frac{(-1)^k}{2k+1} \operatorname{sech}\left((2k+1)\frac{\pi}{2}\rho\right)$$
(2)

where $\rho := a/b$.

A second method using *conformal mappings*, yields

$$\operatorname{arccot} \rho = p(a, b) \frac{\pi}{2} + \operatorname{arg} \mathsf{K} \left(e^{ip(a, b)\pi} \right)$$
(3)

where K is the *complete elliptic integral* of the first kind.

• It will not be apparent to one unfamiliar with inversion of elliptic integrals that (2) and (3) encode the same solution—though they must as the solution is unique in (0,1)—and each can now be used to solve for $\rho = 10$ to arbitrary precision.

*As with the trapezoidal rule, easy can be good.

Enter Srinivasa Ramanujan

Bornemann finally shows that, for far from simple reasons, the answer is

$$p = \frac{2}{\pi} \arcsin(k_{100}),$$
 (4)

where

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

- No one anticipated a closed form like this—a simple composition of Pi, one arcsin and a few square roots.*
- \triangleright Let me show how to finish up the feast.

*Actually fundamental units of real (quadratic/quartic) fields; solutions to Pell's equation.

An apt result in *Pi and the AGM* is that

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \operatorname{sech}\left(\frac{\pi(2n+1)}{2}\rho\right) = \frac{1}{2} \operatorname{arcsin} k, \quad (5)$$

exactly when k_{ρ^2} is parametrized by *theta functions* in terms of the *elliptic nome* as Jacobi discovered.

We have thus gotten

$$k_{\rho^2} = \frac{\theta_2^2(q)}{\theta_3^2(q)} = \frac{\sum_{n=-\infty}^{\infty} q^{(n+1/2)^2}}{\sum_{n=-\infty}^{\infty} q^{n^2}} \qquad q := e^{-\pi\rho}.$$
(6)

Comparing (5) and (2) we see that the solution is $k_{100} = 6.02806910155971082882540712292... 10^{-7}$ as asserted in (4).

- The explicit form follows from 19th century *mod-ular function theory*.
- If only Trefethen had asked for a $\sqrt{210} \times 1$ box, or even better a $\sqrt{15} \times \sqrt{14}$ one.
 - $-k_{15/14}$ and k_{210} share their units (Pi & AGM).

A Singular Interlude

Indeed k_{210} is the *singular value* sent to Hardy in Ramanujan's famous 1913 letter of introduction—ignored by two other famous English mathematicians.

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

matics. Four hours creative work a day is about the limit for a mathematician, he used to say. Lunch, a light meal, in hall. After lunch he loped off for a game of real tennis in the university court. (If it had been summer, he would have walked down to Fenner's to watch cricket.) In the late afternoon, a stroll back to his rooms. That particular day, though, while the timetable wasn't altered, internally things were not going according to plan. At the back of his mind, getting in the way of his complete pleasure in his game, the Indian manuscript nagged away. Wild theorems. Theorems such as he had never seen before, nor imagined. A fraud of genius? A question was forming itself in his mind. As it was Hardy's mind, the question was forming itself with epigrammatic clarity: is a fraud of genius more probable than an unknown mathematician of genius? Clearly the answer was no. Back in his rooms in Trinity, he had another look at the script. He sent word to Littlewood (probably by messenger, certainly not by telephone, for which, like all mechanical contrivances including fountain pens, he had a deep distrust) that they must have a discussion after hall.





That is an occasion at which one would have liked to be present. Hardy, with his combination of remorseless clarity and intellectual panache (he was very English, but in argument he showed the characteristics that Latin minds have often assumed to be their own) : Littlewood, imaginative, powerful, humorous. Apparently it did not take them long. Before midnight they knew, and knew for certain. The writer of these manuscripts was a man of genius. That was as much as they could judge, that night. It was only later that Hardy decided that Ramanujan was, in terms of natural mathematical genius, in the class of Gauss and Euler: but that he could not expect, because of the defects of his education, and because he had come on the scene too late in the line of mathematical history, to make a contribution on the same scale

GH Hardy (1877-1947)

CP Snow's description in *A Mathematician's Apology*

A Modern Finale

Alternatively, armed only with the knowledge that the singular values are always algebraic we may finish with an *au courant* proof: numerically obtain the minimal polynomial from a high precision computation with (6) and recover the surds.

Maple allows the following

- > Digits:=100:with(PolynomialTools):
- > k:=s->evalf(EllipticModulus(exp(-Pi*sqrt(s)))):
- > p:=latex(MinimalPolynomial(k(100),12)):
- > 'Error',fsolve(p)[1]-evalf(k(100)); galois(p);

-106

Error, 4 10

"8T9", {"D(4)[x]2", "E(8):2"}, "+", 16, {"(4 5)(6 7)" 5)(26)(3 7)", "(1 8)(2 3)(4 5)(6 7)", "(2 8)(1 3)(4 6)

This finds the minimal polynomial for k_{100} , checks it to 100 places, tells us the *galois group*, and returns a latex expression 'p' which sets as:

1 - 1658904 $_X$ - 3317540 $_X^2$ + 1657944 $_X^3$ + 6637254 $_X^4$ + 1657944 $_X^5$ - 3317540 $_X^6$ - 1658904 $_X^7$ + $_X^8$, and is *self-reciprocal*: It satisfies $p(x) = x^8 p(1/x)$.

This suggests taking a square root and we discover $y = \sqrt{k_{100}}$ satisfies

$$p(y) = 1 - 1288 y + 20 y^{2} - 1288 y^{3} - 26 y^{4} + 1288 y^{5} + 20 y^{6} + 1288 y^{7} + y^{8}.$$

Now life is good. The prime factors of 100 are 2 and 5 prompting:

subs(_X=z,[op(((factor(p,{sqrt(2),sqrt(5)})))]))

The code yields four quadratic terms, the desired one being

$$q = z^{2} + 322 z - 228 z \sqrt{2} + 144 z \sqrt{5} - 102 z \sqrt{2} \sqrt{5} + 323 - 228 \sqrt{2} + 144 \sqrt{5} - 102 \sqrt{2} \sqrt{5}.$$

For security,

w:=solve(q)[2]: evalf[1000](k(100)-w^2);

gives a 1000-digit error check of $2.20226255 \cdot 10^{-998}$.

• We can work a little more to find, using one of the 3Ms, the beautiful form of k_{100} given in (4).

The Ten Symbolic Challenge Problems

Each of the following requires numeric work—some times considerable—to facilitate whatever transpires thereafter.

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

Extra credit: This constant is an algebraic number of degree not exceeding 20. Find its minimal polynomial.

#2. Evaluate

$$\sum_{(m,n,p)\neq 0} \frac{(-1)^{m+n+p}}{\sqrt{m^2 + n^2 + p^2}},\tag{7}$$

where convergence is over increasingly large cubes surrounding the origin.

Extra credit: Identify this constant.

#3. Evaluate the sum

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

Extra credit: Evaluate this constant as a multiterm expression involving well-known mathematical constants. This expression has seven terms, and involves π , log 2, ζ (3), and Li₅(1/2).

Hint: The expression is "homogenous."

#4. Evaluate

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

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

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



Calculate $R_1(2,2)$.

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

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

Hint: This can be expressed in terms of integrals as

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

Extra credit: Express this constant as a threeterm expression involving algebraic constants and the natural logarithm with an algebraic argument. Similarly:

 #7. Calculate the expected distance between two random points on different faces of the unit cube.
Hint: This can be expressed in terms of integrals

Hint: This can be expressed in terms of integrals as

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

Extra credit: Express this constant as a six-term expression involving algebraic constants and two natural logarithms.

Answers to all ten are detailed in our paper [Bailey, Borwein, Kapoor and Weisstein].

• The final three we finish by further discussing...

#8. Calculate

$$\int_0^\infty \cos(2x) \prod_{n=1}^\infty \cos\left(\frac{x}{n}\right) \, dx. \tag{8}$$

Extra credit: Express this constant as an analytic expression.

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

#9. Calculate

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

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

Solution. In the notation of Lecture II:

$$\zeta(3,1,3,1) = \frac{2\pi^8}{10!},$$

and is the second case of *Zagier's conjecture*, now proven (see APPENDIX I, D).

#10. Evaluate

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

Extra credit: Express this constant in terms of the Gamma function.

History and Context

The challenge of showing that the value of $\pi_2 < \pi/8$ was posed by Bernard Mares, Jr., along with the problem of showing

$$\pi_1 := \int_0^\infty \prod_{n=1}^\infty \cos\left(\frac{x}{n}\right) \, dx < \frac{\pi}{4}.\tag{9}$$

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, due in part to the oscillatory behavior of $\prod_{n\geq 1} \cos(x/n)$ but mostly due to the difficulty of computing high-precision evaluations of the integrand function.

Let f(x) be the integrand function. We can write

$$f(x) = \cos(2x) \left[\prod_{1}^{m} \cos(x/k) \right] \exp(f_m(x)), (10)$$

where we choose m > x, and where

$$f_m(x) = \sum_{k=m+1}^{\infty} \log \cos\left(\frac{x}{k}\right).$$
 (11)
The log cos evaluation can be expanded as follows:

$$\log \cos \left(\frac{x}{k}\right) = \sum_{j=1}^{\infty} \frac{(-1)^j 2^{2j-1} (2^{2j}-1) B_{2j}}{j(2j)!} \left(\frac{x}{k}\right)^{2j},$$

where B_{2j} are *Bernoulli numbers*. Note that since k > m > x in (11), this series converges. We can now write

$$f_m(x) = \sum_{k=m+1}^{\infty} \sum_{j=1}^{\infty} \frac{(-1)^j 2^{2j-1} (2^{2j}-1) B_{2j}}{j(2j)!} \left(\frac{x}{k}\right)^{2j},$$

which after interchanging the sums gives

$$f_m(x) = -\sum_{j=1}^{\infty} \frac{(2^{2j}-1)\zeta(2j)}{j\pi^{2j}} \left[\sum_{k=m+1}^{\infty} \frac{1}{k^{2j}}\right] x^{2j}.$$

or as follows:

$$f_m(x) = -\sum_{j=1}^{\infty} \frac{(2^{2j}-1)\zeta(2j)}{j\pi^{2j}} \left[\zeta(2j) - \sum_{k=1}^m \frac{1}{k^{2j}}\right] x^{2j}.$$

We have more compactly

$$f_m(x) = -\sum_{j=1}^{\infty} a_j b_{j,m} x^{2j},$$

where

$$a_j = \frac{(2^{2j} - 1)\zeta(2j)}{j\pi^{2j}} \quad b_{j,m} = \zeta(2j) - \sum_{k=1}^m 1/k^{2j}.$$
(12)

With this evaluation scheme for f(x) in hand, the integral (8) can be computed using, for instance, the *tanh-sinh quadrature* algorithm, which can be implemented fairly easily on a personal computer or workstation, and which is also well-suited for highly parallel processing .

• This algorithm approximates an integral f(x) on [-1,1] by transforming it to an integral on $(-\infty,\infty)$, using the change of variable x = g(t), where $g(t) = \tanh(\pi/2 \cdot \sinh t)$:

$$\int_{-1}^{1} f(x) dx = \int_{-\infty}^{\infty} f(g(t))g'(t) dt$$
$$= h \sum_{j=-\infty}^{\infty} w_j f(x_j) + E(h). (13)$$

Here $x_j = g(hj)$ and $w_j = g'(hj)$ are abscissas and weights for the tanh-sinh quadrature scheme (which can be pre-computed), and E(h) is the error in this approximation.

• The tanh-sinh quadrature algorithm is designed for a finite integration interval. The simple substitution s = 1/(x+1) reduces again to an integral from 0 to 1. In spite of the substantial precomputation required, the calculation requires only about one minute, using Bailey's *ARPREC* software package The first 100 digits of the result are:

 $\underbrace{0.39269908169872415480783042290993786052464}{5}43418723$ 1595926812285162093247139938546179016512747455366777

The *Inverse Symbolic Calculator*, e.g., suggests this is likely $\pi/8$. But a careful comparison with $\pi/8$:

 $\frac{0.39269908169872415480783042290993786052464}{227621868074038477050785776124828504353167764633497...,}$ reveals they *differ* by approximately 7.407×10^{-43} .

• These two values are provably distinct. The reason is governed by the fact that

$$\sum_{n=1}^{55} \frac{1}{2n+1} > 2 > \sum_{n=1}^{54} \frac{1}{2n+1}.$$

We do not know a concise closed-form evaluation of this constant.

Further History and Context

Recall the *sinc* function

$$\operatorname{sinc}(x) := \frac{\sin(x)}{x}$$

Consider, the seven highly oscillatory integrals below.

$$I_{1} := \int_{0}^{\infty} \operatorname{sinc}(x) dx = \frac{\pi}{2},$$

$$I_{2} := \int_{0}^{\infty} \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) dx = \frac{\pi}{2},$$

$$I_{3} := \int_{0}^{\infty} \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) \operatorname{sinc}\left(\frac{x}{5}\right) dx = \frac{\pi}{2},$$

$$\vdots$$

$$I_{6} := \int_{0}^{\infty} \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{11}\right) dx = \frac{\pi}{2},$$

$$I_{7} := \int_{0}^{\infty} \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{13}\right) dx = \frac{\pi}{2}.$$

However,

$$I_8 := \int_0^\infty \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{15}\right) dx$$
$$= \frac{467807924713440738696537864469}{935615849440640907310521750000}\pi$$

$$\approx$$
 0.49999999992646 π .

- When shown this, a friend using a well-known computer algebra package, and the software vendor concluded there was a "bug" in the software.
- Not so! It is easy to see that the limit of these integrals is $2\pi_1$.

Fourier analysis, via Parseval's theorem, links

$$I_N := \int_0^\infty \operatorname{sinc}(a_1 x) \operatorname{sinc}(a_2 x) \cdots \operatorname{sinc}(a_N x) \, dx$$

with the volume of the polyhedron P_N given by

$$P_N := \{x : |\sum_{k=2}^N a_k x_k| \le a_1, |x_k| \le 1, 2 \le k \le N\},$$

where $x := (x_2, x_3, \cdots, x_N).$

If we let

 $C_N := \{(x_2, x_3, \cdots, x_N) : -1 \le x_k \le 1, 2 \le k \le N\},$ then

$$I_N = \frac{\pi}{2a_1} \frac{\operatorname{Vol}(P_N)}{\operatorname{Vol}(C_N)}.$$

 Thus, the value drops precisely when the constraint

$$\sum_{k=2}^{N} a_k x_k \le a_1$$

becomes *active* and *bites* into the hypercube C_N ; this occurs exactly when $\sum_{k=2}^{N} a_k > a_1$.

• $\frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{13} < 1$, but on addition of $\frac{1}{15}$, the sum exceeds 1, the volume drops, and $I_N = \frac{\pi}{2}$ no longer holds.



Before and after the bite

• A similar analysis applies to π_2 . Moreover, it is fortunate that we began with π_1 or the falsehood of the identity analogous to that displayed above would have been much harder to see.

#10. History and Context

The integral arises in Gaussian and spherical models of ferromagnetism and in the theory of *random walks* (as in extensions of Trefethen #6). It leads to one of the most impressive closed-form evaluations of an equivalent integral due to G.N. Watson:

$$\widehat{W} = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{1}{3 - \cos(x) - \cos(y) - \cos(z)} dx dy dz$$

$$= \frac{1}{96} (\sqrt{3} - 1) \Gamma^2 \left(\frac{1}{24}\right) \Gamma^2 \left(\frac{11}{24}\right) \qquad (14)$$

$$= 4 \pi \left(18 + 12 \sqrt{2} - 10 \sqrt{3} - 7 \sqrt{6}\right) \kappa^2 (k_6),$$

where $k_6 = \left(2 - \sqrt{3}\right) \left(\sqrt{3} - \sqrt{2}\right)$ is the sixth singular value.

The most self contained derivation of this very subtle result is due to Joyce and Zucker.

Solution. We apply the formula

$$\frac{1}{\lambda} = \int_0^\infty e^{-\lambda t} dt, \qquad \operatorname{Re}(\lambda) > 0 \qquad (15)$$

to W_3 . The 3-dimension integral is reducible to a single integral by using

$$\frac{1}{\pi} \int_0^\infty \exp(t \cos \theta) d\theta = I_0(t) \tag{16}$$

is the modified Bessel function of the first kind.

It follows from this that

$$W_3 = \int_0^\infty \exp(-3t) I_0^3(t) dt.$$

which evaluates to arbitrary precision giving:

 $W_3 = 0.505462019717326006052004053227140...$

Finally an integer relation hunt to express $\log W$ in terms of $\log \pi$, $\log 2$, $\log \Gamma(k/24)$ and $\log(\sqrt{3}-1)$ will produce (14).

• We may also write W_3 only as a product of Γ -values.

```
This is what our Mathematician's ToolKit returned:

0= -1.* log[w3] + -1.* log[gamma[1/24]] + 4.*log[gamma[3/24]] +

-8.*log[gamma[5/24]] + 1.* log[gamma[7/24]] +

14.*log[gamma[9/24]]+-6.*log[gamma[11/24]] +

-9.*log[gamma[13/24]] +18.*log[gamma[15/24]] +

-2.*log[gamma[17/24]] +-7.*log[gamma[19/24]]
```

• which is proven by comparing the result with (14) and establishing the implicit Γ - representation of $(\sqrt{3}-1)^2/96$.

- Similar searches suggest there is no similar four dimensional closed form.
- We found that W_4 is not expressible as a product of powers of $\Gamma(k/120)$ (for 0 < k < 120) with coefficients of less than 12 digits.
 - This does not, of course, rule out the possibility of a larger relation, but it does cast doubt, experimentally, that such a relation exists.
 - enough to stop looking!



Advanced Collaborative Environment

CONCLUSION

The many techniques and types of mathematics used are a wonderful advert for multi-field, multi-person, multi-computer, multi-package collaboration.



• Edwards comments in his recent *Essays on Constructive Mathematics* that his own preference for constructivism was forged by experience of computing in the fifties, when computing power was as he notes "trivial by today's standards".

My similar attitudes were cemented primarily by the ability in the early days of personal computers to decode—with the help of APL—exactly the sort of work by Ramanujan which finished #10.

CARATHÉODORY and CHRÉTIEN

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

• Addressing the MAA (retro-digital data-mining?)

A proof is a proof. What kind of a proof? It's a proof. A proof is a proof. And when you have a good proof, it's because it's proven. (Jean Chrétien)

The then Prime Minister, explaining in 2002 how Canada would determine if Iraq had WMDs, sounds a lot like Bertrand Russell!

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APPENDIX I: INTEGER RELATIONS

The USES of LLL and PSLQ

A vector (x_1, x_2, \dots, x_n) of reals *possesses an integer relation* if there are integers a_i not all zero with

$$0 = a_1 x_1 + a_2 x_2 + \dots + a_n x_n.$$

PROBLEM: Find a_i if such exist. If not, obtain lower bounds on the size of possible a_i .

- (n = 2) Euclid's algorithm gives solution.
- $(n \ge 3)$ Euler, Jacobi, Poincare, Minkowski, Perron, others sought method.
- First general algorithm in 1977 by Ferguson & Forcade. Since '77: LLL (in Maple), HJLS, PSOS, PSLQ ('91, parallel '99).

▶ Integer Relation Detection was recently ranked among "the 10 algorithms with the greatest influence on the development and practice of science and engineering in the 20th century." J. Dongarra, F. Sullivan, *Computing in Science & Engineering* **2** (2000), 22–23.

Also: Monte Carlo, Simplex, Krylov Subspace, QR Decomposition, Quicksort, ..., FFT, Fast Multipole Method.

A. ALGEBRAIC NUMBERS

Compute α to sufficiently high precision (O(n^2)) and apply LLL to the vector

$$(1, \alpha, \alpha^2, \cdots, \alpha^{n-1}).$$

- Solution integers a_i are coefficients of a polynomial likely satisfied by α .
- If no relation is found, exclusion bounds are obtained.

B. FINALIZING FORMULAE

▶ If we suspect an identity PSLQ is powerful.

• (Machin's Formula) We try lin_dep on

 $[\arctan(1), \arctan(\frac{1}{5}), \arctan(\frac{1}{239})]$

and recover [1, -4, 1]. That is,

$$\frac{\pi}{4} = 4 \arctan(\frac{1}{5}) - \arctan(\frac{1}{239}).$$

[Used on all serious computations of π from 1706 (100 digits) to 1973 (1 million).]

• (Dase's 'mental' Formula) We try lin_dep on

 $[\arctan(1), \arctan(\frac{1}{2}), \arctan(\frac{1}{5}), \arctan(\frac{1}{8})]$ and recover [-1, 1, 1, 1]. That is,

$$\frac{\pi}{4} = \arctan(\frac{1}{2}) + \arctan(\frac{1}{5}) + \arctan(\frac{1}{8}).$$
[Used by Dase for 200 digits in 1844.]

C. ZETA FUNCTIONS

▶ The *zeta function* is defined, for s > 1, by

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

• Thanks to Apéry (1976) it is well known that

$$S_{2} := \zeta(2) = 3 \sum_{k=1}^{\infty} \frac{1}{k^{2} \binom{2k}{k}}$$
$$A_{3} := \zeta(3) = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^{3} \binom{2k}{k}}$$
$$S_{4} := \zeta(4) = \frac{36}{17} \sum_{k=1}^{\infty} \frac{1}{k^{4} \binom{2k}{k}}$$

► These results *strongly* suggest that

$$\aleph_5 := \zeta(5) / \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^5 \binom{2k}{k}}$$

is a simple rational or algebraic number. Yet, **PSLQ shows**: if \aleph_5 satisfies a polynomial of degree ≤ 25 the Euclidean norm of coefficients *exceeds* 2×10^{37} .

D. ZAGIER'S CONJECTURE

For $r \geq 1$ and $n_1, \ldots, n_r \geq 1$, consider:

$$L(n_1, \ldots, n_r; x) := \sum_{0 < m_r < \ldots < m_1} \frac{x^{m_1}}{m_1^{n_1} \ldots m_r^{n_r}}$$

Thus

$$L(n;x) = \frac{x}{1^n} + \frac{x^2}{2^n} + \frac{x^3}{3^n} + \cdots$$

is the classical polylogarithm, while

$$L(n,m;x) = \frac{1}{1^m} \frac{x^2}{2^n} + \left(\frac{1}{1^m} + \frac{1}{2^m}\right) \frac{x^3}{3^n} + \left(\frac{1}{1^m} + \frac{1}{2^m} + \frac{1}{3^m}\right) \frac{x^4}{4^n} + \cdots,$$

$$L(n,m,l;x) = \frac{1}{1^l} \frac{1}{2^m} \frac{x^3}{3^n} + \left(\frac{1}{1^l} \frac{1}{2^m} + \frac{1}{1^l} \frac{1}{3^m} + \frac{1}{2^l} \frac{1}{3^m}\right) \frac{x^4}{4^n} + \cdots.$$

• The series converge absolutely for |x| < 1 and conditionally on |x| = 1 unless $n_1 = x = 1$.

These polylogarithms

$$L(n_r, \ldots, n_1; x) = \sum_{0 < m_1 < \ldots < m_r} \frac{x^{m_r}}{m_r^{n_r} \ldots m_1^{n_1}},$$

are *determined uniquely* by the **differential equa**tions

$$\frac{d}{dx}L(\mathbf{n_r},\ldots,n_1;x) = \frac{1}{x}L(\mathbf{n_r}-1,\ldots,n_2,n_1;x)$$

if $n_r \ge 2$ and

$$\frac{d}{dx}L(\mathbf{n_r},\ldots,n_2,n_1;x) = \frac{1}{1-x}L(\mathbf{n_{r-1}},\ldots,n_1;x)$$

if $n_r = 1$ with the *initial conditions*

$$L(n_r,\ldots,n_1;0)=0$$

for $r \geq 1$ and

$$L(\emptyset; x) \equiv 1.$$

Set $\overline{s} := (s_1, s_2, \dots, s_N)$. Let $\{\overline{s}\}_n$ denotes concatenation, and $w := \sum s_i$.

Then every *periodic* polylogarithm leads to a function

$$L_{\overline{s}}(x,t) := \sum_{n} L(\{\overline{s}\}_{n}; x)t^{wn}$$

which solves an algebraic ordinary differential equation in x, and leads to nice *recurrences*.

A. In the simplest case, with N = 1, the ODE is $D_sF = t^sF$ where

$$D_s := \left((1-x) \frac{d}{dx} \right)^1 \left(x \frac{d}{dx} \right)^{s-1}$$

and the solution (by series) is a generalized hypergeometric function:

$$L_{\overline{s}}(x,t) = 1 + \sum_{n \ge 1} x^n \frac{t^s}{n^s} \prod_{k=1}^{n-1} \left(1 + \frac{t^s}{k^s} \right),$$

as follows from considering $D_s(x^n)$.

B. Similarly, for N = 1 and negative integers

$$L_{\overline{-s}}(x,t) := 1 + \sum_{n \ge 1} (-x)^n \frac{t^s}{n^s} \prod_{k=1}^{n-1} \left(1 + (-1)^k \frac{t^s}{k^s} \right),$$

and $L_{-1}(2x-1,t)$ solves a hypergeometric ODE.

► Indeed

$$L_{\overline{-1}}(1,t) = \frac{1}{\beta(1+\frac{t}{2},\frac{1}{2}-\frac{t}{2})}$$

C. We may obtain ODEs for eventually periodic Euler sums. Thus, $L_{-2,1}(x,t)$ is a solution of

$$t^{6} F = x^{2}(x-1)^{2}(x+1)^{2} D^{6} F$$

+ $x(x-1)(x+1)(15x^{2}-6x-7) D^{5} F$
+ $(x-1)(65x^{3}+14x^{2}-41x-8) D^{4} F$
+ $(x-1)(90x^{2}-11x-27) D^{3} F$
+ $(x-1)(31x-10) D^{2} F + (x-1) DF.$

• This leads to a four-term recursion for $F = \sum c_n(t)x^n$ with initial values $c_0 = 1, c_1 = 0, c_2 = t^3/4, c_3 = -t^3/6$, and the ODE can be simplified.

We are now ready to prove Zagier's conjecture. Let F(a, b; c; x) denote the *hypergeometric function*. Then:

Theorem 1 (BBGL) For |x|, |t| < 1 and integer $n \ge 1$

$$\sum_{n=0}^{\infty} L(\underbrace{3,1,3,1,\ldots,3,1}_{n-fold};x) t^{4n}$$

$$= F\left(\frac{t(1+i)}{2}, \frac{-t(1+i)}{2};1;x\right)$$
(17)
$$\times F\left(\frac{t(1-i)}{2}, \frac{-t(1-i)}{2};1;x\right).$$

Proof. Both sides of the putative identity start

$$1 + \frac{t^4}{8}x^2 + \frac{t^4}{18}x^3 + \frac{t^8 + 44t^4}{1536}x^4 + \cdots$$

and are *annihilated* by the differential operator

$$D_{31} := \left((1-x) \frac{d}{dx} \right)^2 \left(x \frac{d}{dx} \right)^2 - t^4.$$

 Once discovered — and it was discovered after much computational evidence — this can be checked variously in Mathematica or Maple (e.g., in the package gfun)!

Corollary 2 (Zagier Conjecture)

$$\zeta(\underbrace{3,1,3,1,\ldots,3,1}_{n-fold}) = \frac{2\pi^{4n}}{(4n+2)!}$$
(18)

QED

Proof. We have

$$F(a, -a; 1; 1) = \frac{1}{\Gamma(1-a)\Gamma(1+a)} = \frac{\sin \pi a}{\pi a}$$

where the first equality comes from Gauss's evaluation of F(a, b; c; 1).

Hence, setting x = 1, in (17) produces

$$F\left(\frac{t(1+i)}{2}, \frac{-t(1+i)}{2}; 1; 1\right) F\left(\frac{t(1-i)}{2}, \frac{-t(1-i)}{2}; 1; 1\right)$$
$$= \frac{2}{\pi^2 t^2} \sin\left(\frac{1+i}{2}\pi t\right) \sin\left(\frac{1-i}{2}\pi t\right)$$
$$= \frac{\cosh \pi t - \cos \pi t}{\pi^2 t^2} = \sum_{n=0}^{\infty} \frac{2\pi^{4n} t^{4n}}{(4n+2)!}$$

on using the Taylor series of cos and cosh. Comparing coefficients in (17) ends the proof. QED

- What other deep Clausen-like hypergeometric factorizations lurk within?
- If one suspects that (2) holds, once one can compute these sums well, it is easy to verify many cases numerically and be entirely convinced.
- ♠ This is the *unique* non-commutative analogue of Euler's evaluation of $\zeta(2n)$.

APPENDIX II. MATHEMATICAL MODELS



The New York Cimes

Mathematical Form 0006

Kuen's surface: constant negative curvature.



Hiroshi Sugimoto for The New York Times

Felix Klein's heritage

Considerable obstacles generally present themselves to the beginner, in studying the elements of Solid Geometry, from the practice which has hitherto uniformly prevailed in this country, of never submitting to the eye of the student, the figures on whose properties he is reasoning, but of drawing perspective representations of them upon a plane. ... I hope that I shall never be obliged to have recourse to a perspective drawing of any figure whose parts are not in the same plane. Augustus de Morgan (1806– 71).



- First President of the LMS, he was equally influential as an educator and a researcher
- There is evidence young children see more naturally in three than two dimensions



Donald Coxeter's (1907–2003) **octahedral kaleidoscope** built in Liverpool (circa 1925)



4D Coxeter polytope with 120 dodecahedral faces



 In a 1997 paper, Coxeter showed his friend M.C. Escher, knowing no math, had achieved "mathematical perfection" in etching *Circle Limit III*. "Escher did it by instinct," Coxeter wrote, "I did it by trigonometry."

David Mumford recently noted that Donald Coxeter placed great value on working out details of complicated explicit examples: In my book, Coxeter has been one of the most important 20th century mathematicians *—not because he started a new perspective,* but because he deepened and extended so beautifully an older esthetic. The classical goal of geometry is the exploration and enumeration of geometric configurations of all kinds, their symmetries and the constructions relating them to each other. The goal is not especially to prove theorems but to discover these perfect objects and, in doing this, theorems are only a tool that imperfect humans need to reassure themselves that they have seen them correctly. (David Mumford, 2003)

20th C. MATHEMATICAL MODELS



Ferguson's "Eight-Fold Way" sculpture

The Fergusons won the 2002 Communications Award, of the Joint Policy Board of Mathematics. The citation runs:



They have dazzled the mathematical community and a far wider public with exquisite sculptures embodying mathematical ideas, along with artful and accessible essays and lectures elucidating the mathematical concepts.

It has been known for some time that the *hyperbolic* volume V of the **figure-eight knot complement** is

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

= 2.029883212819307250042405108549...



Ferguson's "Figure-Eight Knot Complement" sculpture

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

$$C_j = \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n (6n+j)^2}.$$
 (19)



Indeed, as Broadhurst found, using PSLQ (*Fergu-son's Integer Relation Algorithm*):

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

- Entering the following code in the *Mathematician's Toolkit*, at **www.expmath.info**:
 - 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}]]
```

recovers the solution vector

(9, -18, 18, 24, 6, -2, 0)

- The *first proof* that this formula holds is given in our recent book
- The formula is inscribed on each cast of the sculpture marrying both sides of Helaman!

21st C. MATHEMATICAL MODELS



Knots 10_{161} (L) and 10_{162} (C) agree (R)*



In a NewMedia Cave or Plato's?

*KnotPlot: from Little (1899) to Perko (1974) and on

Experimental Mathematics:

Apéry-Like Identities for $\zeta(n)$

Jonathan M. Borwein, FRSC

Research Chair in IT Dalhousie University

Halifax, Nova Scotia, Canada

2005 Clifford Lecture IV

Tulane, March 31–April 2, 2005

We wish to consider one of the most fascinating and glamorous functions of analysis, the Riemann zeta function. (R. Bellman)

Siegel found several pages of ... numerical calculations with ... zeroes of the zeta function calculated to several decimal places each. As Andrew Granville has observed "So much for pure thought alone." (JB & DHB)



AK Peters 2004

Talk Revised: 03–29–05


Website disclaimers

Brookhaven National Labs on Long Island, NY, had to put up a disclaimer on their website that the world is actually still safe after it got out that they created a mini black hole by slamming together two gold nuclei at 99.9995 the speed of light. Should go down in the annuals of 'website disclaimers' and a rare bit of nerd speak, marketing and Douglas Adams "Don't Panic".

At http://www.bnl.gov click on <u>Black holes at RHIC?</u> The back hole is quite beautiful see http://www.chem.cmu.edu/images/photos/mkev2smallfront.jpg

Steve DiPaola, School of Interactive Arts & Technology, SFU www.dipaola.org www.dipaola.org/gallery

Apéry-Like Identities for $\zeta(n)$

The final lecture comprises a research level case study of generating functions for zeta functions. This lecture is based on past research with David Bradley and current research with David Bailey.

One example is

$$\begin{aligned} \mathcal{Z}(x) &:= 3 \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k} (k^2 - x^2)} \prod_{n=1}^{k-1} \frac{4x^2 - n^2}{x^2 - n^2} \\ &= \sum_{n=1}^{\infty} \frac{1}{n^2 - x^2} \\ &= \sum_{k=0}^{\infty} \zeta(2k+2) x^{2k} = \frac{1 - \pi x \cot(\pi x)}{2x^2} \end{aligned}$$
(1)

Note that with x = 0 this recovers

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

Riemann's Original 1859 Manuscript

Mender to sold de Pringelle and - ever gigibras Grocer. his deter (Boden chosehel wille, 1859, Non what) des hargent orden et angegeten hiert gendent. Dere Gesting geste and her ber Mi der Berten (0) fingeten beletig en ersteren der geste der Soller werden und für der ersteren der der er og anneret gester verster genden Text alle der er og anneret der Ster mighten genden Text alle on angeden sol som des te typel, der genten Bei angeben Grimme stert, typel, der genten Bei angeben Grimme stert, and regeten und er Gesten gester Grimme stert, and regeten und er Gesten gester Sterten anderster topel angeben der Gester gester ander anderster and regeten und er Gesten gester ander anderster topen angeben der Gester gester ander anderster anderster topen angeben der Gester andere andere andere sollte sollte andere sollte soll Aure Dans for dre Anyoritany, will so woor das her dense dand dos defeature ander the Corresponde An hat you That werden la seco, glande set and beden des and for evening of the day of fit and the line of the fit of the day of fit and the day of the mylen Grissen And enstreed a Astresse, adder Games and Divices demalle langere for governant hal , and caller hiter to go will not go you works and int. Ad and berte and use Horizone Das Fadaged daler and the time day and and all gradges the dress lector sending dreske one's als Angen prince doe von later gemache Benerning Pour de Podes der tel grale myster and trace low Are gen $\mathcal{T} - \frac{1}{1 - \frac{1}{1+\delta}} = \frac{2}{n\delta},$ Matyral - de la ne nitri al - int = (-n. tai) (-20) man fir polle Prompalla, fir nolle garge- Tallin Len . M(0-1) . & (0) = (20) Z . " ((-i)" + i "), greatly wind . Du Fundor der & mysleren korsater ale me helder prode 2(0) ~ 2(1. 0) welde wit _____ heady of here to grant for a tope det to the TT and so and rank to 2 (0) liken a, well dened den bet dismins, colonge At convergence, daugestills word, by a se sol durch S(0). But any in my a by andle That but the and the stand of the st and grieseral list; estind and mansheilt on in gills buches And men do Prechow ford - David A mention der gamens 1 2 - mx a-1 dx - JI(0-1) der That had a can ense menzoniched $\frac{1}{n^{\alpha}} \overline{\pi} \begin{pmatrix} \alpha \\ i \end{pmatrix}, \overline{\pi}^{-\frac{1}{2}} \int_{e^{-i\pi \frac{1}{2}\pi x}}^{\infty} \frac{4}{dx}.$ Montest and and so the transfer alus, bear men ge entre = 4(x) pertol, T(=-1). # = 2(0) = J Y(x) x + dx, J GAD da . . . 24(1)+1 = x 2(24(1)+1), (Fardi, F.D. S. 184) nort a bio to position on frienderstras T(2-1) == 2310 - J W (x) x = 1 dx + J 4(+) x = dx + + / (x + x + -) da whe dot to show a dorden Fit youly we make $=\frac{1}{A(e-1)}+\int_{-\infty}^{\infty}\psi(x)\left(x^{\frac{6}{4}-1}+x^{-\frac{1+6}{4}}\right)dx.$ men anderts, a enjite and dream bies gland (e- voi e Tei) f " tota , romagnety , den or der vielent og Turchora Tos when new s = ' + ti and 可(き)(カー) = ちくの)= きけ), (-x) = ela-11 l's(-x) d . Ly - te - x as bost - 1 word ist, doss er fin in regulioux seell wind have

- Showing the *Euler product* and the *reflection* formula (s → 1 − s). Even the notation is as today.
 - As seen recently on Numb3rs and Law and Order— ζ is starting to compete with π .

Jegelener Gringellen under ernen (Boden charabe mille, 1859 Non what) here Dans fis dre Angeichung, welles wer das her dents dend dir defeature when the Conceptorde An hel yo That worken la see, glands ich and beston deducer on encouring of my daws it wand - hid word estalline Extentions hald got getread machineters the Merchang ever best menting where do dis figrent der Prinzahle; en Gegendan), welsten dires das Arresse, alleter Games - I Diricles demalle lingere for good and hal , and aredan hitsen by vielenes will goog and the motion. the docsor lader and ing docate our als through my Jewned die von Ealer gemachte Bamerrany, Von de Product more fir polle Promyalla, fir nolle gamp- Tallen geach and . Dre Function der Engelenen her Sater laken s, will devel den berte during, colorge At convergine, dangestills word by a se ich durch S(0). But any in my a by der selle That was a grisserale tool; estind and markenets on the Assending dar Generas 1 e - ma a - de - T(0-1) enally man y minted JI (0-1) . \$ (0) = 1 at de franket men un dis Feligrel J Gast de vorten bis + a prosition en fringebil entral works durt - iter and orders for yrabour on Tamer and sill, so engicht and dream hirst gland (e - nei e Tai) / x de



George Friedrich Bernard Riemann (1826-1866)

The Riemann Hypothesis

 $\mathcal{G} \lor \mathcal{L} \lor \dots$ The only Millennium and Hilbert Problem



All non-real zeros have real part 'one half'

★★ Note the monotonicity of $x \mapsto |\zeta(x+iy)|$.

This is equivalent to (RH) as discovered in 2002^{*}.

*By Zvengerowski and Saidal in a complex analysis class.

ODLYZKO and the NON-TRIVIAL ZEROS

Andrew Odlyzko: Tables of zeros of the Riemann zeta function

- The first 100,000 zeros of the Riemann zeta function, accurate to within 3*10^(-9). [text, 1.8 MB] [gzip'd text, 730 KB]
- The first 100 zeros of the Riemann zeta function, accurate to over 1000 decimal places. [text]
- Zeros number 10^12+1 through 10^12+10^4 of the Riemann zeta function. [text]
- Zeros number 10^21+1 through 10^21+10^4 of the Riemann zeta function. [text]
- Zeros number 10^22+1 through 10^22+10^4 of the Riemann zeta function. [text]

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14.13472514221.02203963925.01085758030.42487612632.93506158837.58617815940.91871901243.327073281



▶ The imaginary parts of the first 8 zeroes; they do lie on the critical line.
 ▶ At 10²² the Law of small numbers still rules.
 ▶ Real zeroes are at -2N /www.dtc.umn.edu/~odlyzko/

An ELEMENTARY WARMUP

The well known series for \arcsin^2 generalizes fully:

Theorem. For $|x| \leq 2$ and $N = 1, 2, \ldots$

$$\frac{\operatorname{arcsin}^{2N}\left(\frac{x}{2}\right)}{(2N)!} = \sum_{k=1}^{\infty} \frac{H_N(k)}{\binom{2k}{k}k^2} x^{2k}, \qquad (3)$$

where $H_1(k) = 1/4$ and

$$H_{N+1}(k) := \sum_{n_1=1}^{k-1} \frac{1}{(2n_1)^2} \sum_{n_2=1}^{n_1-1} \frac{1}{(2n_2)^2} \cdots \sum_{n_N=1}^{n_{N-1}-1} \frac{1}{(2n_N)^2},$$

and

$$\frac{\arcsin^{2N+1}\left(\frac{x}{2}\right)}{(2N+1)!} = \sum_{k=0}^{\infty} \frac{G_N(k)\binom{2k}{k}}{2(2k+1)4^{2k}} x^{2k+1}, \quad (4)$$

where $G_0(k) = 1$ and

$$G_N(k) := \sum_{n_1=0}^{k-1} \frac{1}{(2n_1+1)^2} \sum_{n_2=0}^{n_1-1} \frac{1}{(2n_2+1)^2} \cdots \sum_{n_N=0}^{n_{N-1}-1} \frac{1}{(2n_N+1)^2}.$$

► Thus, for N = 1, 2, ... [N = 1 recovers (2)] $\infty H_N(k) = \pi^{2N}$

$$\sum_{k=1}^{N} \frac{\pi_N(\kappa)}{\binom{2k}{k}k^2} = \frac{\pi}{6^{2N}(2N)!}.$$
$$\left[\frac{1}{72}\pi^2, \frac{1}{31104}\pi^4, \frac{1}{33592320}\pi^6, \frac{1}{67722117120}\pi^8\right]$$

BINOMIAL SUMS and PSLQ

 \blacktriangleright Any relatively prime integers p and q such that

$$\zeta(5) \stackrel{?}{=} \frac{p}{q} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5 \binom{2k}{k}}$$

have q astronomically large (as "lattice basis reduction" shows).

► But ··· PSLQ yields in *polylogarithms*:

$$A_{5} = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^{5} \binom{2k}{k}} = 2\zeta(5)$$

- $\frac{4}{3}L^{5} + \frac{8}{3}L^{3}\zeta(2) + 4L^{2}\zeta(3)$
+ $80 \sum_{n>0} \left(\frac{1}{(2n)^{5}} - \frac{L}{(2n)^{4}}\right) \rho^{2n}$

where

$$L := \log(\rho)$$

and

$$\rho := (\sqrt{5} - 1)/2$$

with similar formulae for A_4, A_6, S_5, S_6 and S_7 .

- A less known formula for $\zeta(5)$ due to Koecher suggested generalizations for $\zeta(7), \zeta(9), \zeta(11)...$
- Again the coefficients were found by integer relation algorithms. *Bootstrapping* the earlier pattern kept the search space of manageable size.
- For example, and simpler than Koecher:

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

► We were able – by finding integer relations for n = 1, 2, ..., 10 – to encapsulate the formulae for $\zeta(4n + 3)$ in a single conjectured generating function, (entirely *ex machina*).

► The discovery was:

Theorem 1 For any complex z,

$$\sum_{n=0}^{\infty} \zeta(4n+3)z^{4n}$$

$$= \sum_{k=1}^{\infty} \frac{1}{k^3(1-z^4/k^4)}$$

$$= \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^3\binom{2k}{k}(1-z^4/k^4)} \prod_{m=1}^{k-1} \frac{1+4z^4/m^4}{1-z^4/m^4}.$$
(6)

- The first '=' is easy. The second is quite unexpected in its form.
- Setting z = 0 yields Apéry's formula for $\zeta(3)$ and the coefficient of z^4 is (14).

$$\left|\sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k\binom{2k}{k}} = \frac{2}{\sqrt{5}} \log\left(\frac{1+\sqrt{5}}{2}\right)\right|$$

(7)

HOW IT WAS FOUND

▶ The first ten cases show (6) has the form

$$rac{5}{2} \sum_{k \geq 1} rac{(-1)^{k-1}}{k^3 \binom{2k}{k}} rac{P_k(z)}{(1-z^4/k^4)}$$

for *undetermined* P_k ; with abundant data to compute

$$P_k(z) = \prod_{m=1}^{k-1} \frac{1 + 4z^4/m^4}{1 - z^4/m^4}.$$

• We found many reformulations of (6), including a marvellous **finite** sum:

$$\sum_{k=1}^{n} \frac{2n^2}{k^2} \frac{\prod_{i=1}^{n-1} (4k^4 + i^4)}{\prod_{i=1, i \neq k}^{n} (k^4 - i^4)} = \binom{2n}{n}.$$
 (8)

 Obtained via Gosper's (Wilf-Zeilberger type) telescoping algorithm after a mistake in an electronic Petri dish ('infty' ≠ 'infinity').

- ► This finite identity was subsequently proved by Almkvist and Granville (*Experimental Math*, 1999) thus finishing the proof of (6) and giving a rapidly converging series for any $\zeta(4N + 3)$ where N is positive integer.
- ★ Perhaps shedding light on the irrationality of $\zeta(7)$?

Recall that $\zeta(2N + 1)$ is not proven irrational for N > 1. One of $\zeta(2n + 3)$ for n = 1, 2, 3, 4 is irrational (Rivoal et al).



Kakeya's needle was an excellent false conjecture

PAUL ERDŐS (1913-1996)

Paul Erdős, when shown (8) shortly before his death, rushed off.



Twenty minutes later he returned saying he did not know how to prove it but if proven it would have implications for Apéry's result (' ζ (3) is irrational').

The CURRENT RESEARCH

• We now document the discovery of two generating functions for $\zeta(2n + 2)$, analogous to earlier work for $\zeta(2n + 1)$ and $\zeta(4n + 3)$, initiated by Koecher and completed by various other authors.

Recall: an *integer relation relation algorithm* is an algorithm that, given n real numbers (x_1, x_2, \dots, x_n) , finds integers a_i such that

$$a_1x_1 + a_2x_2 + \dots + a_nx_n = 0,$$

at least to within available numerical precision, or else establishes that there are no integers a_i within a ball of radius A—in the Euclidean norm:

$$A = (a_1^2 + a_2^2 + \dots + a_n^2)^{1/2}.$$

- Helaman Ferguson's "PSLQ" is the most widely known integer relation algorithm, although variants of the "LLL" algorithm are also well used.
- © Such algorithms are now the basis of the the "Recognize" function in *Mathematica* and of the "identify" function in *Maple*, and form the basis of our work.

The existence of series formulas involving central binomial coefficients in the denominators for the ζ(2), ζ(3), and ζ(4)—and the role of the formula for ζ(3) in Apéry's proof of its irrationality —has prompted considerable effort to extend these results to larger integer arguments.

The formulas in question are

$$\zeta(2) = 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k}}, \qquad (9)$$

$$\zeta(3) = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^3 \binom{2k}{k}},$$
 (10)

$$\zeta(4) = \frac{36}{17} \sum_{k=1}^{\infty} \frac{1}{k^4 \binom{2k}{k}}.$$
 (11)

(9) has been known since the 19C—it relates to $\arcsin^2(x)$ —while (10) was variously discovered in the 20C and (11) was proved by Comptet. These three are the only single term identities or "seeds".

• A coherent proof of all three was provided by Borwein-Broadhurst-Kamnitzer in course of a more general study of such central binomial series and so called *multi-Clausen sums*. These results make it tempting to conjecture

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

is a simple rational or algebraic number.

Example. Integer relation shed light on \mathfrak{Q}_5 .

- **1997** If \mathfrak{Q}_5 is algebraic of degree 24 then the Euclidean norm of coefficients exceeds 2×10^{37} .
- 2005 Using 10,000-digit precision, the norm exceeds $1.24\times10^{383}.$
- **2005** If $\zeta(5)$ is algebraic of degree 24 its norm exceeds 1.98×10^{380} .

Moreover, a study of *polylogarithmic ladders in the* golden ratio (BBK), produced

$$2\zeta(5) - \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5 \binom{2k}{k}} = \frac{5}{2} \operatorname{Li}_5(\rho) - \frac{5}{2} \operatorname{Li}_4(\rho) \ln \rho + \zeta(3) \log^2 \rho - \frac{1}{3} \zeta(2) \log^3 \rho - \frac{1}{24} \log^5 \rho, \quad (12)$$

where $\rho = (3-\sqrt{5})/2$ and where $\text{Li}_N(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^N}$ is the *polylogarithm* of order N.

- Since the terms on the right hand side are almost certainly algebraically independent, we see how unlikely it is that Q_5 is rational.
- We note that at present it is proven only that one of $\zeta(5), \zeta(7), \zeta(9), \zeta(11)$ is irrational; and that a nontrivial density of all odd values is.

Given the negative result from PSLQ computations for \mathfrak{Q}_5 , Bradley and JMB systematically investigated the possibility of a multi-term identity of this general form for $\zeta(2n+1)$.

The following was then recovered early in experimental searches using computer-based integer relation tools:

$$\zeta(5) = 2\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5 \binom{2k}{k}} - \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^2}$$
(13)

▶ In a similar way, identities were found for $\zeta(7), \zeta(9)$ and $\zeta(11)$ (the identity for $\zeta(9)$ is listed later):

$$\begin{aligned} \zeta(7) &= \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^7 \binom{2k}{k}} + \frac{25}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} \\ (14) \\ \zeta(11) &= \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^{11} \binom{2k}{k}} + \frac{25}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^7 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} \\ &- \frac{75}{4} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^8} \\ &+ \frac{125}{4} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} \sum_{i=1}^{k-1} \frac{1}{i^4}. \end{aligned}$$
(15)

- Note that the formulas for ζ(7) and ζ(11) include, as the first term, a close analogue of the formula for ζ(3) given above, and the first two coefficients in (15) clearly repeat those in (14).
 - this suggested that a "bootstrap" approach might allow production of enough higher-level formulas for $\zeta(4n+3)$ for $m = 2, 3, \cdots$ to determine the closed form:

- Indeed, this was the case; in fact, such "bootstrapping" helped by restricting the number of multiple relations that otherwise makes the analysis difficult or impossible.
 - we were able to sum all higher variables up to k-1 which significantly speeds up numerical computation
- such issues have, so far, prevented the generalization of formulas such as the one above for ζ(5) to the general case of ζ(4n + 1)

The following general formula, due to Koecher following techniques of Knopp and Schur,

$$\frac{1}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{\binom{2k}{k} k^3} \frac{5k^2 - x^2}{k^2 - x^2} \prod_{n=1}^{k-1} \left(1 - \frac{x^2}{n^2}\right)$$
$$= \sum_{n=1}^{\infty} \frac{1}{n\left(n^2 - x^2\right)}.$$
(16)

gives (13) as its second term but more complicated expressions for $\zeta(7)$ and $\zeta(11)$ than (14) and (15).

After bootstrapping, 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, produced the following remarkable result:

$$\frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^3 \binom{2k}{k} (1 - x^4/k^4)} \prod_{m=1}^{k-1} \left(\frac{1 + 4x^4/m^4}{1 - x^4/m^4} \right)$$
$$= \sum_{n=0}^{\infty} \zeta (4n+3) x^{4n} = \sum_{k=1}^{\infty} \frac{1}{k^3 (1 - x^4/k^4)}$$
(17)

 rigorously established by Almkvist-Granville, it can now be handled in part symbolically by Wilf-Zeilberger (WZ) methods

It is also the x = 0 case of the unified formula *conjectured by Cohen after much experiment* (Rivoal, 2005):

$$\frac{1}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k\binom{2k}{k}} \frac{5k^2 - x^2}{k^4 - x^2k^2 - y^4} \times \prod_{n=1}^{k-1} \frac{(n^2 - x^2)^2 + 4y^4}{n^4 - x^2n^2 - y^4} = \sum_{n=1}^{\infty} \frac{n}{n^4 - x^2n^2 - y^4}$$
(18)

 \sim

in which setting y = 0 recovers (16).

 Stimulated by Rivoal's paper, we decided to revisit the even ζ-values.

An analogous, but more deliberate, experimental procedure, as detailed below yielded a formula for $\zeta(2n+2)$ that is pleasingly parallel to (17):

$$3\sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k} \left(1 - x^2/k^2\right)} \prod_{m=1}^{k-1} \left(\frac{1 - 4x^2/m^2}{1 - x^2/m^2}\right)$$
$$= \sum_{n=0}^{\infty} \zeta \left(2n + 2\right) x^{2n} = \sum_{m=1}^{\infty} \frac{1}{\left(m^2 - x^2\right)}$$
(19)
$$= \frac{\pi \cot(\pi x) x - 1}{x^2}.$$



OCR and Touch

 \triangleright We finish by discussing the existence of a formula based on the seed $\zeta(4)$, and like questions. The Details for $\zeta(2n+2)$

▷ We applied a similar though distinct experimental approach to produce a generating function for $\zeta(2n+2)$. We describe this process of discovery in some detail as the general technique appears to be quite fruitful.

Conjecture: $\zeta(2n+2)$ is a rational combination of terms of the form

$$\sigma(2r; [2a_1, \cdots, 2a_N]) := \sum_{k > n_i > 0} \frac{1}{k^{2r} \binom{2k}{k} \prod_{i=1}^N n_i^{2a_i}},$$
(20)

where $r + \sum_{i=1}^{N} a_i = n + 1$, and the a_i are listed in nonincreasing order

- RHS is independent of the order of the a_i

One can then write

$$Z(x) := \sum_{n=0}^{\infty} \zeta(2n+2) x^{2n}$$
(21)
=
$$\sum_{n=0}^{\infty} \sum_{r=1}^{\infty} \sum_{\pi \in \Pi(n-r)} \alpha(k,\pi) \sigma(2r;2\pi) x^{2r+2(n-r)},$$

as $\Pi(m)$ ranges over *additive partitions* of m.

Write $\alpha(\pi) := \alpha(0, \pi)$ and define $\hat{\sigma}_k([\cdot]) := 1$ for the null partition $[\cdot]$, and, for a partition $\pi = (\pi_1, \pi_2, \dots, \pi_N)$ of m > 0, written in nonincreasing order,

$$\hat{\sigma}_k(\pi) := \sum_{k > n_i > 0} \frac{1}{n_i^{2\pi_1} \cdots n_N^{2\pi_N}}.$$
(22)

▶ The α 's appear to be independent of k:

$$Z(x) = \sum_{n=0}^{\infty} \sum_{r=1}^{\infty} \sum_{\pi \in \Pi(n-r)}^{\infty} \alpha(\pi) \,\sigma(2r; 2\pi) x^{2r+2(n-r)}$$

$$= \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}} \sum_{r=0}^{\infty} \frac{x^{2r}}{k^{2r+2}} \sum_{m=0}^{n-1} \sum_{\Pi(m)} \alpha(\pi) \hat{\sigma}_k(\pi) x^{2m}$$

$$= \sum_{k \ge 1} \frac{1}{\binom{2k}{k} (k^2 - x^2)} P_k(x)$$

for functions $P_1, P_2, \ldots, P_k, \ldots$ whose form must be determined.

• Crucially we compute that for some $\gamma_{k,m}$

$$P_{k}(x) = \sum_{m \ge 0} \gamma_{k,m} x^{2m}$$
(23)
$$= \sum_{m=0}^{\infty} \left\{ \sum_{\pi \in \Pi(m)} \alpha(\pi) \sum_{n_{i} < k} \frac{1}{n_{i}^{2\pi_{1}} \cdots n_{N}^{2\pi_{N}}} \right\} x^{2m}$$

- ★ Our strategy is to compute the first few explicit cases of $P_k(x)$, and hope they permit us to extrapolate the closed form, much as in the case of $\zeta(4n+3)$.
 - Some examples we produced are shown below. At each step we "bootstrapped," noting that certain coefficients of the current result are the coefficients of the previous result.
 - we found the remaining coefficients by integer relation computations
 - In particular, we computed high-precision (200digit) numerical values of the assumed terms and the left-hand-side zeta value, and then applied PSLQ to find the rational coefficients.
 - in each case we "hard-wired" the first few coefficients to agree with the coefficients of the preceding formula

- 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 terms (with coefficients in bold) are followed by terms for the other partitions
 - 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):

$$\begin{split} \zeta(2) &= 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}k^2} = 3\sigma(2,[0]), \\ \zeta(4) &= 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}k^4} - 9\sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k-1} j^{-2}}{\binom{2k}{k}k^2} = 3\sigma(4,[0]) - 9\sigma(2,[2]) \\ \zeta(6) &= 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}k^6} - 9\sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k-1} j^{-2}}{\binom{2k}{k}k^4} - \frac{45}{2}\sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k-1} j^{-4}}{\binom{2k}{k}k^2} \\ &+ \frac{27}{2}\sum_{k=1}^{\infty} \sum_{j=1}^{k-1} \frac{\sum_{i=1}^{i-1} i^{-2}}{j^2\binom{2k}{k}k^2}, \\ &= 3\sigma(6,[]) - 9\sigma(4,[2]) - \frac{45}{2}\sigma(2,[4]) + \frac{27}{2}\sigma(2,[2,2]) \\ \zeta(8) &= 3\sigma(8,[]) - 9\sigma(6,[2]) - \frac{45}{2}\sigma(4,[4]) + \frac{27}{2}\sigma(4,[2,2]) \\ &- 63\sigma(2,[6]) + \frac{135}{2}\sigma(2,[4,2]) - \frac{27}{2}\sigma(2,[2,2,2]) \\ \zeta(10) &= 3\sigma(10,[]) - 9\sigma(8,[2]) - \frac{45}{2}\sigma(6,[4]) + \frac{27}{2}\sigma(6,[2,2]) \\ &- 63\sigma(4,[6]) + \frac{135}{2}\sigma(4,[4,2]) - \frac{27}{2}\sigma(4,[2,2,2]) \\ &- \frac{765}{4}\sigma(2,[8]) + 189\sigma(2,[6,2]) + \frac{675}{8}\sigma(2,[4,4]) \\ &- \frac{405}{4}\sigma(2,[4,2,2]) + \frac{81}{8}\sigma(2,[2,2,2,2]), \end{split}$$

• From the above results, one can immediately read that $\alpha([\cdot]) = 3$, $\alpha([1]) = -9$, $\alpha([2]) = -45/2$, $\alpha([1,1]) = 27/2$, and so forth.

Table 1 presents the values of α that we obtained in this manner.

Partition	α	Partition	α	Partition	α
[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	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	-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	-1458/64
1 1	2187/4480				

Alpha coefficients found by PSLQ

 Using these results, we use formula (23) to calculate series approximations—to order 17— for the functions P_k(x):

$$\begin{array}{ll} P_{3}(x) &\approx & 3-\frac{45}{4}x^{2}-\frac{45}{16}x^{4}-\frac{45}{64}x^{6}-\frac{45}{256}x^{8}-\frac{45}{1024}x^{10}-\frac{45}{4096}x^{12}-\frac{45}{16384}x^{14}\\ &-\frac{45}{65536}x^{16}\\ P_{4}(x) &\approx & 3-\frac{49}{9}x^{2}+\frac{119}{144}x^{4}+\frac{3311}{5184}x^{4}+\frac{38759}{186624}x^{6}+\frac{384671}{6718464}x^{8}\\ &+\frac{3605399}{241864704}x^{10}+\frac{33022031}{8707129344}x^{12}+\frac{299492039}{313456656384}x^{14}\\ P_{5}(x) &\approx & 3-\frac{205}{16}x^{2}+\frac{7115}{2304}x^{4}+\frac{207395}{331776}x^{6}+\frac{4160315}{47775744}x^{8}+\frac{74142995}{6879707136}x^{10}\\ &+\frac{1254489515}{20542695432781824}x^{12}+\frac{20685646595}{142657607172096}x^{14}\\ &+\frac{36694674715}{20542695432781824}x^{16}\\ P_{6}(x) &\approx & 3-\frac{5269}{400}x^{2}+\frac{6640139}{1440000}x^{4}+\frac{1635326891}{518400000}x^{6}-\frac{5944880821}{18662400000000}x^{8}\\ &-\frac{212874252291349}{671846400000000000}x^{10}-\frac{141436384956907381}{2418647040000000000000}x^{12}\\ &-\frac{70524260274859115989}{131345665638400000000000000}x^{14}\\ &-\frac{31533457168819214655541}{6718464000000000}x^{6}-\frac{680040118121}{8662400000000}x^{8}\\ &-\frac{278500311775049}{6718464000000000}x^{10}-\frac{84136715217872681}{2418647040000000000000}x^{12}\\ &-\frac{22363377813883431689}{87071293440000000000000}x^{16}\\ &-\frac{278500311775049}{87071293440000000000000}x^{10}-\frac{84136715217872681}{24186470400000000000000}x^{12}\\ &-\frac{22363377813883431689}{8707129344000000000000000}x^{16}\\ &-\frac{5560090840263911428841}{31345665638400000000000000000000}x^{16}\\ \end{array}$$

• With these approximations in hand, we attempt to determine closed-form expressions for $P_k(x)$.

This can be done by using either "*Pade*" function in either *Mathematica* or *Maple*.

We obtained the following values*:

$$P_{1}(x) = 3$$

$$P_{2}(x) = \frac{3(4x^{2} - 1)}{(x^{2} - 1)}$$

$$P_{3}(x) = \frac{12(4x^{2} - 1)}{(x^{2} - 4)}$$

$$P_{4}(x) = \frac{12(4x^{2} - 1)(4x^{2} - 9)}{(x^{2} - 4)(x^{2} - 9)}$$

$$P_{5}(x) = \frac{48(4x^{2} - 1)(4x^{2} - 9)}{(x^{2} - 9)(x^{2} - 16)}$$

$$P_{6}(x) = \frac{48(4x^{2} - 1)(4x^{2} - 9)(4x^{2} - 25)}{(x^{2} - 9)(x^{2} - 16)(x^{2} - 25)}$$

$$P_{7}(x) = \frac{192(4x^{2} - 1)(4x^{2} - 9)(4x^{2} - 25)}{(x^{2} - 16)(x^{2} - 25)(x^{2} - 36)}$$

- These results immediately predict the general form of a generating function identity:
- *A bug in first alpha run gave a more complicated numerator for P_5 !

$$\mathcal{Z}(x) = 3 \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k} (k^2 - x^2)} \prod_{n=1}^{k-1} \frac{4x^2 - n^2}{x^2 - n^2}$$
(24)
$$= \sum_{k=0}^{\infty} \zeta(2k+2) x^{2k} = \sum_{n=1}^{\infty} \frac{1}{n^2 - x^2}$$

$$= \frac{1 - \pi x \cot(\pi x)}{2x^2}$$
(25)

We have confirmed this result in several ways:

- 1. Symbolically computing the series coefficients of the LHS and the RHS of (25), and have verified that they agree up to the term with x^{100} .
- 2. We verified that $\mathcal{Z}(1/6)$, computing using (24), agrees with $18-3\sqrt{3}\pi$, computed using (25), to over 2,500 digit precision; likewise for $\mathcal{Z}(1/2) =$ 2, $\mathcal{Z}(1/3) = 9/2 - 3\pi/(2\sqrt{3}), \ \mathcal{Z}(1/4) = 8 - 2\pi$ and $\mathcal{Z}(1/\sqrt{2}) = 1 - \pi/\sqrt{2} \cdot \cot(\pi/\sqrt{2}).$
- 3. We then *checked* that formula (24) gives the same numerical value as (25) for the 100 *pseudo-random values* $\{m\pi\}$, for $1 \le m \le 100$, where $\{\cdot\}$ denotes fractional part.

A Computational Proof

 Identity (24)–(25) can be proven by the methods of Rivoal's recent paper, which combine those in Borwein-Bradley and Almkvist-Granville. This relies on the *equivalent* finite identity:

$$3n^2 \sum_{k=n+1}^{2n} \frac{\prod_{m=n+1}^{k-1} \frac{4n^2 - m^2}{n^2 - m^2}}{\binom{2k}{k} \left(k^2 - n^2\right)} = \frac{1}{\binom{2n}{n}} - \frac{1}{\binom{3n}{n}}$$

- we rewrite (26) as

$$_{3}\mathsf{F}_{2}\left(\begin{array}{c}3n,n+1,-n\\2n+1,n+1/2\end{array};\frac{1}{4}\right) = \frac{\binom{2n}{n}}{\binom{3n}{n}}.$$
 (26)

and set $P(n) = {}_{3}\mathsf{F}_{2} \begin{pmatrix} 3n, n+1, -n \\ 2n+1, n+1/2 \end{pmatrix}$; $\frac{1}{4}$, $R(n) = {\binom{2n}{n}}/{\binom{3n}{n}}$. Then P(0) = 1 = R(0) while $\frac{P(n+1)}{P(n)} = \frac{4(2n+1)^{2}}{3(3n+2)(3n+1)} = \frac{R(n+1)}{R(n)}$, where *Maple* or WZ gives the simplification.

- thus, *inductively* P(n) = R(n) for all n.

• We have proven (26).

QED

The Details for $\zeta(2n+4)$

We have likewise now obtained for the *third seed*:

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

the generating function

$$\mathcal{W}(x) = \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k} k^2} \frac{1}{k^2 - x^2} \prod_{n=1}^{k-1} \left(1 - \frac{x^2}{n^2} \right)$$

$$= \sum_{k=1}^{\infty} \frac{1}{(2k)!} \frac{\prod_{n=1}^{k-1} \left(n^2 - x^2 \right)}{k^2 - x^2} \qquad (27)$$

$$= \sum_{n=0}^{\infty} \gamma_n \zeta(2n+4) x^{2n} \qquad (28)$$

$$\stackrel{?}{=} \alpha_0 \sum_{n=1}^{\infty} \frac{1}{n^4} \mathcal{R}\left(\frac{x^2}{n^2}\right) \qquad (29)$$

where the coefficients γ_n are again computable rational numbers:

$$\mathcal{W}(x) = \frac{17}{36}\zeta(4) + \frac{313}{648}\zeta(6)x^2 + \frac{23147}{46656}\zeta(8)x^4 + \frac{1047709}{2099520}\zeta(10)x^6 + O\left(x^8\right).$$

• We observe that for integers, η_{2n} ,

$$\gamma_{2n} = \frac{\eta_{2n}}{6^{2n-2}\operatorname{numer}(\mathsf{B}_{2n})}.$$

- this suggest that perhaps we are looking at multiples of arcsin(1/2) not Zeta values.

Indeed,

$$\sigma(2; [\underbrace{2, \cdots, 2}_{N-1}]) = \frac{(\pi/3)^{2N}}{(2N)!},$$

for $N \geq 1$.

• The η_{2n} values begin

 $17, 626, 23147, 4190836, 20880863207 \dots$

We aim so to determine the form of the function \mathcal{R} . The anticipated form is along the lines of (16), (18), and (19).

1. First, suppose \mathcal{R} is *rational of degree* N in x^2 :

$$\mathcal{R}_N(x) = \sum_{m=1}^{2N} \frac{\alpha_m}{\beta_m - x}, \qquad \mathcal{R}_N^{(j)}(0) = \sum_{m=1}^{2N} \frac{j! \, \alpha_m}{(\beta_m)^{j+1}},$$

having $\mathcal{R}_N(0) = 1$, and with coefficients determined by

$$\mathcal{W}^{(2j)}(0) = (2j-1)! \gamma_{2j} \zeta(2j+4) = \alpha_0 \mathcal{R}_N^{(2j)}(0) \zeta(2j+4).$$

Thus, $\alpha_0 = 17/36$ and the conditions to be met are that for some N

$$\gamma_j = \frac{17}{36} \sum_{m=1}^{2N} \frac{\alpha_m}{(\beta_m)^{j+1}}$$

for $j = 1, 2, ..., N$ with $\gamma_{2j+1} \equiv 0$.

- this does not *appear* to be solvable
- 2. We next look for a rational *poly-exponential* generating function in which

$$\mathcal{R}_N(x) = \frac{\sum_{i=1}^N p_i(x) e^{\lambda_i x}}{\sum_{i=1}^N q_i(x) e^{\mu_i x}},$$

for polynomials p_i, q_i and scalars λ_i, μ_i , as is the case for the *Bernoulli numbers* $(t/(\exp(t) - 1))$, *Euler numbers* $(2 \operatorname{sech}(x))$ and on.

CONCLUDING COMMENTS

We believe that this general experimental procedure will ultimately yield results for yet other classes of arguments, such as for $\zeta(4n+m)$, m = 0 or m = 1, but our current experimental results are negative.

I. Considering $\zeta(4n+1)$, for n = 9 the simplest evaluation we know is

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

This is one term shorter than the 'new' identity for $\zeta(9)$ given by Rivoal, which comes from taking the coefficient of $x^2 y^4$ in (18). **II.** For $\zeta(2n + 4)$ (and $\zeta(4n)$) starting with (11) which we again recall:

$$\zeta(4) = \frac{36 \cdot 1}{17} \sum_{k=1}^{\infty} \frac{1}{k^4 \binom{2k}{k}},$$

the identity for $\zeta(6)$ most susceptible to bootstrapping is

$$\zeta(6) = \frac{36 \cdot 8}{163} \left[\sum_{k=1}^{\infty} \frac{1}{k^6 \binom{2k}{k}} + \frac{3}{2} \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} \right]$$

• For $\zeta(8)$ —and $\zeta(10)$ —we have enticingly found:

$$\zeta(8) = \frac{36 \cdot 64}{1373} \left[\sum_{k=1}^{\infty} \frac{1}{k^8 \binom{2k}{k}} + \frac{9}{4} \sum_{k=1}^{\infty} \frac{1}{k^4 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} + \frac{3}{2} \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^6} \right]$$

- but this pattern is not fruitful; it stops after one more case (n = 10).
Enter RAMANUJAN Again

Hyperbolic series connect $\zeta(2N+1)$ and π^{2N+1}

• For
$$M \equiv -1 \pmod{4}$$

 $\zeta(4N+3) = -2\sum_{k\geq 1} \frac{1}{k^{4N+3}(e^{2\pi k}-1)}$

$$+\frac{2}{\pi}\left\{\frac{4N+7}{4}\zeta(4N+4)-\sum_{k=1}^{N}\zeta(4k)\zeta(4N+4-4k)\right\}$$

where the interesting term is the hyperbolic series.

• Correspondingly, for $M \equiv 1 \pmod{4}$

$$\zeta(4N+1) = -\frac{2}{N} \sum_{k \ge 1} \frac{(\pi k + N)e^{2\pi k} - N}{k^{4N+1}(e^{2\pi k} - 1)^2}$$

$$+\frac{1}{2N\pi}\Big\{(2N+1)\zeta(4N+2)+\sum_{k=1}^{2N}(-1)^{k}2k\zeta(2k)\zeta(4N+2-2k)\Big\}.$$

- Only a finite set of $\zeta(2N)$ values is required and the full precision value e^{π} is reused throughout.
- $◊ e^{\pi}$ is the easiest transcendental to fast compute (by elliptic methods). One "differentiates" $e^{-s\pi}$ to obtain π (via the AGM iteration).

• For $\zeta(4N + 1)$, I decoded "nicer" series from a couple of PSLQ observations by Simon Plouffe.

THEOREM. For
$$N = 1, 2, \ldots$$

$$\left\{2 - (-4)^{-N}\right\} \sum_{k=1}^{\infty} \frac{\coth(k\pi)}{k^{4N+1}} - (-4)^{-2N} \sum_{k=1}^{\infty} \frac{\tanh(k\pi)}{k^{4N+1}} = Q_N \times \pi^{4N+1}, \quad (30)$$

where the quantity Q_N in (30) is an explicit rational:

$$Q_N := \sum_{k=0}^{2N+1} \frac{B_{4N+2-2k}B_{2k}}{(4N+2-2k)!(2k)!} \\ \times \left\{ (-1)^{\binom{k}{2}} (-4)^N 2^k + (-4)^k \right\}.$$

• On substituting

$$tanh(x) = 1 - \frac{2}{\exp(2x) + 1}$$

and

$$\operatorname{coth}(x) = 1 + \frac{2}{\exp(2x) - 1}$$

one may solve for

$$\zeta(4N+1).$$

 $\star\star$ We finish with 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

$$\zeta(9) = \frac{125}{3704778} \pi^9 - \frac{2}{495} \sum_{k=1}^{\infty} \frac{1}{(1+e^{2k\pi})k^9} + \frac{992}{495} \sum_{k=1}^{\infty} \frac{1}{(1-e^{2k\pi})k^9}$$

- Will we ever identify universal formulae like (30) automatically? My work was highly human aided.
- How do we connect these to the binomial sums?



Knots, Pens and Cameras

CARL FRIEDRICH GAUSS

 Boris Stoicheff's often enthralling biography of Herzberg* records Gauss writing:



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

Carl Friedrich Gauss (1777-1855)



*Gerhard Herzberg (1903-99) fled Germany for Saskatchewan in 1935 and won the 1971 Chemistry Nobel

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