Mathematics by Experiment, I & II:

Plausible Reasoning in the 21st Century

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`www.cecm.sfu.ca/~jborwein/talks.html`

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Abstract. *In the first of these two lectures I shall talk generally about experimental mathematics. In Part II, I shall present some more detailed and sophisticated examples.*

The emergence of powerful mathematical computing environments, the growing availability of correspondingly powerful (multi-processor) computers and the pervasive presence of the internet allow for research mathematicians, students and teachers, to proceed heuristically and 'quasi-inductively'. We may increasingly use symbolic and numeric computation visualization tools, simulation and data mining.

Many of the benefits of computation are accessible through low-end 'electronic blackboard' versions of experimental mathematics [1, 8]. This also permits livelier classes, more realistic examples, and more collaborative learning. Moreover, the distinction between computing (HPC) and communicating (HPN) is increasingly moot.

The unique features of our discipline make this both more problematic and more challenging. For example, there is still no truly satisfactory way of displaying mathematical notation on the web; and we care more about the reliability of our literature than does any other science. **The traditional role of proof in mathematics is arguably under siege.**

Limned by examples, I intend to pose questions ([9]) such as:

- What constitutes secure mathematical knowledge?

- When is computation convincing? Are humans less fallible?

- What tools are available? What methodologies?

- What about the ‘law of the small numbers’?

- How is mathematics actually done? How should it be?

- Who cares for certainty? What is the role of proof?

And I shall offer some personal conclusions.

Many of the 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 friends [2, 3].

They often rely on the sophisticated use of *Integer Relations Algorithms* — recently ranked among the 'top ten' algorithms of the century [7, 8]. (See [4, 5] and `www.cecm.sfu.ca/projects/IntegerRelations/`.)

- As time permits, I shall also describe **WestGrid**, the new Western Canadian computer grid (`www.westgrid.ca`), and my own advanced collaboration facility, **CoLab** (`www.colab.sfu.ca`).

Part II—Experimentation in Mathematics:

Computational Paths to Discovery

Part I—Mathematics by Experiment:

Plausible Reasoning in the 21st Century

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SIMON and RUSSELL

"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.

[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."

GAUSS and HADAMARD

Gauss once confessed,

"I have the result, but I do not yet know how to get it."

◇ Issac Asimov and J. A. Shulman, ed., *Isaac Asimov's Book of Science and Nature Quotations*, Weidenfield and Nicolson, New York, 1988, pg. 115.

...

"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.

MOTIVATION and GOAL

INSIGHT – demands speed $\equiv$ parallelism

- For rapid verification.
- For validation; proofs *and* refutations.
- For "monster barring".

† What is "easy" changes while HPC and HPN blur; merging disciplines and collaborators.

- Parallelism $\equiv$ more space, speed & stuff.
- Exact $\equiv$ hybrid $\equiv$ symbolic '+' numeric (MapleVI meets NAG).
- For analysis, algebra, geometry & topology.

COMMENTS

- Towards an Experimental **Mathodology** — philosophy and practice.

- Intuition is acquired — mesh computation and mathematics.

- Visualization — three is a lot of dimensions.

- "Caging" and "Monster-barring" (Lakatos).

  - graphic checks: compare $2\sqrt{y} - y$ and $\sqrt{y}\ln(y)$, $0 < y < 1$

  - randomized checks: equations, linear algebra, primality

PART of OUR ‘METHODOLOGY’

1. (*High Precision*) computation of object(s).

2. *Pattern Recognition* of *Real Numbers* (Inverse Calculator and ’RevEng’)*, or *Sequences* (Salvy & Zimmermann’s ‘gfun’, Sloane and Plouffe’s Encyclopedia).

3. Extensive use of ‘Integer Relation Methods’: *PSLQ* & *LLL* and FFT.†

   - Exclusion bounds are especially useful.

   - Great test bed for “Experimental Math”.

4. Some automated theorem proving (Wilf-Zeilberger etc).

*ISC space limits: from 10Mb in 1985 to 10Gb today.

†Top Ten “Algorithm’s for the Ages,” Random Samples, Science, Feb. 4, 2000.

FOUR EXPERIMENTS

• 1. **Kantian** example: generating "the classical non-Euclidean geometries (hyperbolic, elliptic) by replacing Euclid's axiom of parallels (or something equivalent to it) with alternative forms."

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

• 3. **Aristotelian** demonstrations: "apply electrodes to a frog's sciatic nerve, and lo, the leg kicks; always precede the presentation of the dog's dinner with the ringing of a bell, and lo, the bell alone will soon make the dog dribble."

• 4. 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."

◇ It is also the only one of the four forms which will make Experimental Mathematics a serious enterprise.

• From Peter Medawar's *Advice to a Young Scientist*, Harper (1979).

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."

...

- Consider the following images of zeroes of 0/1 polynomials
`www.cecm.sfu.ca/MRG/INTERFACES.html`

◇ But symbols are often more reliable than pictures.

On to the examples ...

I: GENERAL EXAMPLES

1. TWO INTEGRALS

- A. $\pi \neq \frac{22}{7}$.

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

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

$$\cdots$$

- *B. The sophomore's dream.*

$$\int_0^1 \frac{1}{x^x}\,dx = \sum_{n=1}^{\infty} \frac{1}{n^n}.$$

2. TWO INFINITE PRODUCTS

- *A. a rational evaluation*:

$$\prod_{n=2}^{\infty} \frac{n^3 - 1}{n^3 + 1} = \frac{2}{3}$$

$$\ldots$$

- *B. and a transcendent one*:

$$\prod_{n=2}^{\infty} \frac{n^2 - 1}{n^2 + 1} = \frac{\pi}{\sinh(\pi)}$$

3. HIGH PRECISION FRAUD

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

is valid to 268 places; while

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

is valid to just 12 places.

- Both are actually transcendental numbers.

Correspondingly the *simple continued fractions* for $\tanh(\pi)$ and $\tanh(\frac{\pi}{2})$ are respectively

$$[0, 1, \mathbf{267}, 4, 14, 1, 2, 1, 2, 2, 1, 2, 3, 8, 3, 1]$$

and

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

- Bill Gosper describes how continued fractions let you "see" what a number is. "[I]t's completely astounding ... it looks like you are cheating God somehow."

4. PARTIAL FRACTIONS & CONVEXITY

• We consider a network *objective function* p_N given by

$$p_N(\vec{q}) = \sum_{\sigma \in S_N} (\prod_{i=1}^{N} \frac{q_{\sigma(i)}}{\sum_{j=i}^{N} q_{\sigma(j)}})(\sum_{i=1}^{N} \frac{1}{\sum_{j=i}^{N} q_{\sigma(j)}})$$

summed over *all* $N!$ permutations; so a typical term is

$$(\prod_{i=1}^{N} \frac{q_i}{\sum_{j=i}^{N} q_j})(\sum_{i=1}^{N} \frac{1}{\sum_{j=i}^{n} q_j}) \ .$$

◇ For $N = 3$ this is

$$q_1 q_2 q_3 (\frac{1}{q_1 + q_2 + q_3})(\frac{1}{q_2 + q_3})(\frac{1}{q_3})$$

$$\times(\frac{1}{q_1 + q_2 + q_3} + \frac{1}{q_2 + q_3} + \frac{1}{q_3}) \ .$$

- We wish to show p_N is *convex* on the positive orthant. First we try to simplify the expression for p_N.

• The *partial fraction decomposition* gives:

$$\begin{aligned}
p_1(x_1) &= \frac{1}{x_1}, \\
p_2(x_1, x_2) &= \frac{1}{x_1} + \frac{1}{x_2} - \frac{1}{x_1 + x_2}, \\
p_3(x_1, x_2, x_3) &= \frac{1}{x_1} + \frac{1}{x_2} + \frac{1}{x_3} \\
&- \frac{1}{x_1 + x_2} - \frac{1}{x_2 + x_3} - \frac{1}{x_1 + x_3} \\
&+ \frac{1}{x_1 + x_2 + x_3}.
\end{aligned}$$

So we predict the 'same' for $N = 4$ and we:

CONJECTURE. For each $N \in \mathbb{N}$

$$p_N(x_1, \ldots, x_N) \ := \ \int_0^1 \left(1 - \prod_{i=1}^{N} (1 - t^{x_i})\right) \frac{dt}{t}$$

is convex, indeed 1/concave.

- One may prove this for $N < 6$ via a large symbolic Hessian – and make many 'random' numerical checks.

PROOF. A year later, interpreting the original function as a *joint expectation* of Poisson distributions gave:

$$p_N(\vec{x}) = \int_{\mathbb{R}^n_+} e^{-(y_1+\cdots+y_n)} \max\left(\frac{\mathbf{y_1}}{\mathbf{x_1}}, \ldots, \frac{\mathbf{y_n}}{\mathbf{x_n}}\right) dy.$$

- See *SIAM Electronic Problems and Solutions.* `www.siam.org/journals/problems/`

5. CONVEX CONJUGATES and NMR

The *Hoch and Stern information measure*, or *neg-entropy*, is defined in complex $n-$space by

$$H(z) = \sum_{j=1}^{n} h(z_j/b),$$

where h is convex and given (for scaling b) by:

$$\boxed{h(z) \triangleq |z| \ln\left(|z| + \sqrt{1+|z|^2}\right) - \sqrt{1+|z|^2}}$$

for quantum theoretic (NMR) reasons.

- Recall the *Fenchel-Legendre conjugate*

$$f^*(y) := \sup_x \langle y, x\rangle - f(x).$$

- Our *symbolic convex analysis* package (stored at `www.cecm.sfu.ca/projects/CCA/`) produced:

$$h^*(z) = \cosh(|z|)$$

◇ Compare the *Shannon entropy*:

$$(z \ln z - z)^* = \exp(z).$$

$\diamond$ I'd never have tried by hand!

• Efficient *dual algorithms* now may be constructed.

$\diamond$ Knowing 'closed forms' helps:

$$(\exp\exp)^*(y) = y\ln(y) - y\{W(y) + W(y)^{-1}\}$$

where Maple or Mathematica knows the complex *Lambert* W function

$$W(x)e^{W(x)} = x.$$

Thus, the conjugate's series is

$$-1+(\ln(y)-1)\,y-\frac{1}{2}y^2+\frac{1}{3}y^3-\frac{3}{8}y^4+\frac{8}{15}y^5+O\left(y^6\right).$$

Coworkers: Marechal, Naugler, $\cdots$, Bauschke, Fee, Lucet

6. SOME FOURIER INTEGRALS

Recall the *sinc* function

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

Consider, the seven highly oscillatory integrals below.*

$$I_1 := \int_0^\infty \mathrm{sinc}(x)\, dx = \frac{\pi}{2},$$

$$I_2 := \int_0^\infty \mathrm{sinc}(x)\mathrm{sinc}\left(\frac{x}{3}\right)\, dx = \frac{\pi}{2},$$

$$I_3 := \int_0^\infty \mathrm{sinc}(x)\mathrm{sinc}\left(\frac{x}{3}\right)\mathrm{sinc}\left(\frac{x}{5}\right)\, dx = \frac{\pi}{2},$$

$$\cdots$$

$$I_6 := \int_0^\infty \mathrm{sinc}(x)\mathrm{sinc}\left(\frac{x}{3}\right)\cdots\mathrm{sinc}\left(\frac{x}{11}\right)\, dx = \frac{\pi}{2},$$

$$I_7 := \int_0^\infty \mathrm{sinc}(x)\mathrm{sinc}\left(\frac{x}{3}\right)\cdots\mathrm{sinc}\left(\frac{x}{13}\right)\, dx = \frac{\pi}{2}.$$

*These are hard to compute accurately numerically.

However,

$$I_8 := \int_0^\infty \mathrm{sinc}(x)\mathrm{sinc}\left(\frac{x}{3}\right)\cdots\mathrm{sinc}\left(\frac{x}{15}\right)\,dx$$

$$= \frac{467807924713440738696537864469}{935615849440640907310521750000}\pi$$

$$\approx 0.499999999992646\pi.$$

• When a researcher, using a well-known computer algebra package, checked this he – and the makers – concluded there was a "bug" in the software. Not so!

◇ Our analysis, via Parseval's theorem, links the integral

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

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

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

• Thus, the value drops precisely when the constraint $\sum_{k=2}^{N} a_k x_k \le a_1$ becomes *active* and bites the hypercube C_N. That occurs when

$$\sum_{k=2}^{N} a_k > a_1.$$

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

- A somewhat cautionary example for too enthusiastically inferring patterns from seemingly compelling symbolic or numerical computation.

Coworkers: D. Borwein, Mares

7. MINIMAL POLYNOMIALS

of COMBINATORIAL MATRICES

Consider matrices A, B, C, M:

$$A_{kj} := (-1)^{k+1}\binom{2n-j}{2n-k},$$

$$B_{kj} := (-1)^{k+1}\binom{2n-j}{k-1},$$

$$C_{kj} := (-1)^{k+1}\binom{j-1}{k-1}$$

$(k, j = 1, \ldots, n)$ and

$$\boxed{M := A + B - C.}$$

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

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

• The key is discovering

$$(1) \qquad \begin{aligned} A^2 &= C^2 = I \\ B^2 &= CA, \qquad AC = B. \end{aligned}$$

• It follows that $B^3 = BCA = AA = I$, and that the *group generated by* A,B and C is S_3.

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

• One now easily shows using (1)

$$\boxed{M^2 + M = 2I}$$

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

$$`minpoly(B, x)` \ldots$$

- Random matrices have full degree *minimal polynomials*.

- *Jordan Forms* uncover Spectral Abscissas.

Coworkers: D. Borwein, Girgensohn.

8. PARTITIONS and PATTERNS

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

$$\prod_{n\geq 1}(1-q^n)^{-1}.$$

$\diamond$ Thus $p(5)=7$ since

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

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

QUESTION. How hard is $p(n)$ to compute – in 1900 (for MacMahon), and 2000 (for Maple)?

...

• *Euler's pentagonal number theorem* is

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

$\diamond$ We can recognize the *triangular numbers* in *Sloane's* on-line 'Encyclopedia of Integer Sequences'. And much more.

9. ESTABLISHING INEQUALITIES

and the MAXIMUM PRINCIPLE

• Consider the two *means*

$$\mathcal{L}^{-1}(x,y) := \frac{x-y}{\ln(x)-\ln(y)}$$

and

$$\mathcal{M}(x,y) := \sqrt[\frac{3}{2}]{\frac{x^{\frac{2}{3}}+y^{\frac{2}{3}}}{2}}$$

• An *elliptic integral* estimate reduced to the elementary inequalities

$$\boxed{\mathcal{L}(\mathcal{M}(x,1),\sqrt{x}) < \mathcal{L}(x,1) < \mathcal{L}(\mathcal{M}(x,1),1)}$$

for $0 < x < 1$.

⋄ We first discuss a method of showing

$$\mathcal{E}(x) := \mathcal{L}(x,1) - \mathcal{L}(\mathcal{M}(x,1),\sqrt{x}) > 0$$

on $0 < x < 1$.

A. Numeric/symbolic methods

- $\lim_{x \to 0+} \mathcal{E}(x) = \infty$.

- *Newton-like iteration* shows that $\mathcal{E}(x) > 0$ on $[0.0, 0.9]$.

- *Taylor series* shows $\mathcal{E}(x)$ has 4 zeroes at 1.

- *Maximum Principle* shows there are no more zeroes inside $C := \{z : |z - 1| = \frac{1}{4}\}$:

$$\frac{1}{2\pi i} \int_C \frac{\mathcal{E}'}{\mathcal{E}} = \#(\mathcal{E}^{-1}(0); C)$$

- When we make each step *effective*.

B. Graphic/symbolic methods

Consider the ‘opposite’ (cruder) inequality

$$\mathcal{F}(x) := \mathcal{L}(\mathcal{M}(x,1),1) - \mathcal{L}(x,1) > 0$$

- Then we may observe that it holds since
  - $\mathcal{M}$ is a mean; and
  - $\mathcal{L}$ is decreasing.

BERLINSKI

"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."

...

"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."

II. π and FRIENDS

A: (*A quartic algorithm.*) Set $a_0 = 6 - 4\sqrt{2}$ and $y_0 = \sqrt{2} - 1$. Iterate

$$y_{k+1} = \frac{1 - (1 - y_k^4)^{1/4}}{1 + (1 - y_k^4)^{1/4}}$$

$$\begin{aligned} a_{k+1} &= a_k(1 + y_{k+1})^4 \\ &- 2^{2k+3} y_{k+1}(1 + y_{k+1} + y_{k+1}^2) \end{aligned}$$

Then a_k converges *quartically* to $1/\pi$.

• Used since 1986, with Salamin-Brent scheme, by Bailey, Kanada (Tokyo).

• In 1997, Kanada computed over 51 billion digits on a Hitachi supercomputer (18 iterations, 25 hrs on 2^{10} cpu's), and 2^{36} digits in April 1999.

In December 2002, Kanada computed π to over **1.24 trillion decimal digits**. His team first computed π in hexadecimal (base 16) to 1,030,700,000,000 places, using the following two arctangent relations:

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

$$\pi = 176 \tan^{-1} \frac{1}{57} + 28 \tan^{-1} \frac{1}{239} - 48 \tan^{-1} \frac{1}{682} + 96 \tan^{-1} \frac{1}{12943}$$

• Kanada verified the results of these two computations agreed, and then converted the hex digit sequence to decimal and back.

◇ A billion (2^{30}) digit computation has been performed on a single Pentium II PC in under 9 days.

◇ 50 billionth decimal digit of π *or* $\frac{1}{\pi}$ is 04$\underline{2}$! And after 17 billion digits 0123456789 has finally appeared (Brouwer's famous intuitionist example *now* converges!).

<u>Details at</u>: www.cecm.sfu.ca/personal/jborwein/pi_cover.html.

B: (A *nonic (ninth-order) algorithm.*) In 1995 Garvan and I found genuine η-based m-th order approximations to π.

$\diamond$ Set

$$a_0 = 1/3,\ r_0 = (\sqrt{3}-1)/2,\ s_0 = \sqrt[3]{1-r_0^3}$$

and iterate

$$\begin{aligned} t &= 1+2r_k & \quad u &= [9r_k(1+r_k+r_k^2)]^{1/3} \\ v &= t^2+tu+u^2 & \quad m &= \frac{27(1+s_k+s_k^2)}{v} \\ s_{k+1} &= \frac{(1-r_k)^3}{(t+2u)v} & \quad r_{k+1} &= (1-s_k^3)^{1/3} \end{aligned}$$

and

$$a_{k+1} = ma_k + 3^{2k-1}(1-m)$$

Then $1/a_k$ converges *nonically* to π.

• Their discovery and proof both used enormous amounts of computer algebra (e.g., hunting for '$\sum \Rightarrow \prod$' and 'the modular machine')

† Higher order schemes are slower than quartic.

• Kanada's estimate of time to run the same FFT/Karatsuba-based π algorithm on a serial machine: *"infinite"*.

Coworkers: Bailey, P. Borwein, Garvan, Kanada, Lisoněk

C: (*'Pentium farming' for binary digits.*) Bailey, P. Borwein and Plouffe (1996) discovered a series for π (and some other *polylogarithmic constants*) which allows one to compute hex–digits of π *without* computing prior digits.

• The algorithm needs very little memory and does not need multiple precision. The running time grows only slightly faster than linearly in the order of the digit being computed.

• The key, found by 'PSLQ' (below) is:

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

• Knowing an algorithm would follow they spent several months hunting for such a formula.

$\diamond$ Once found, easy to prove in Mathematica, Maple or by hand.

$\diamond$ A most successful case of

REVERSE MATHEMATICAL ENGINEERING

• (Sept 97) Fabrice Bellard (INRIA) used a variant formula to compute 152 binary digits of π, starting at the *trillionth position* (10^{12}). This took 12 days on 20 work-stations working in parallel over the Internet.

• (August 98) Colin Percival (SFU, age 17) finished a similar 'embarassingly parallel' computation of *five trillionth bit* (using 25 machines at about 10 times the speed). In *Hex*:

$$\underline{0}7E45733CC790B5B5979$$

The binary digits of π starting at the 40 trillionth place are

$$\underline{0}00001111110011111.$$

• (September 00) The quadrillionth bit is '0' (used 250 cpu years on 1734 machines in 56 countries). From the $999,999,999,999,997$th bit of π one has:

$$111000110001000010110101100000110$$

⋄ One of the largest computations ever!

• Bailey and Crandall (2001) make a reasonable, hence very hard conjecture, about the **uniform distribution of a related chaotic dynamical system**. This conjecture implies:

Existence of a 'BBP' formula in base b for an irrational α ensures the normality base b of α.

For $\log 2$ the dynamical system is

$$x_{n+1} \equiv 2(x_n + \frac{1}{n}) \mod 1,$$

`www.sciencenews.org/20010901/bob9.asp`.

• In any given base, $\arctan(\frac{p}{q})$ has a BBP formula for a dense set of rationals.

D: (*Other polylogarithms.*) Catalan's constant

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

is not proven irrational.

• In a series of inspired computations using *polylogarithmic ladders* Broadhurst has since found – and proved – similar identities for constants such as $\zeta(3)$, $\zeta(5)$ and G. Broadhurst's binary formula is

$$\begin{aligned} G = 3 \sum_{k=0}^{\infty} \frac{1}{2 \cdot 16^k} & \left\{ \frac{1}{(8k+1)^2} - \frac{1}{(8k+2)^2} \right. \\ + & \quad \frac{1}{2(8k+3)^2} - \frac{1}{2^2(8k+5)^2} \\ + & \quad \left. \frac{1}{2^2(8k+6)^2} - \frac{1}{2^3(8k+7)^2} \right\} \\ + & \end{aligned}$$

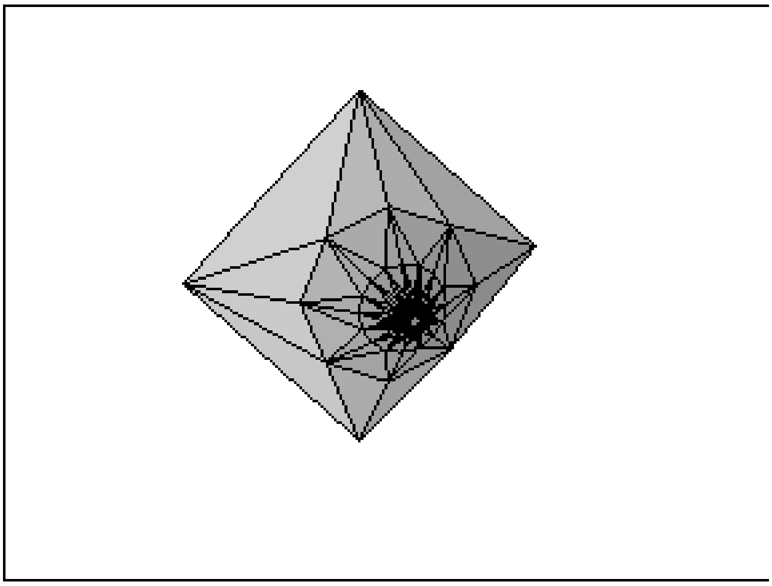
$$-2\sum_{k=0}^{\infty}\frac{1}{8\cdot 16^{3k}}\left\{\begin{array}{cl} & \dfrac{1}{(8k+1)^2}+\dfrac{1}{2(8k+2)^2} \\ + & \dfrac{1}{2^3(8k+3)^2}-\dfrac{1}{2^6(8k+5)^2} \\ - & \dfrac{1}{2^7(8k+6)^2}-\dfrac{1}{2^9(8k+7)^2}\end{array}\right\}$$

- Why was G missed earlier?

- He also gives some constants with ternary expansions.

Coworkers: BBP, Bellard, Broadhurst, Percival, the Web, $\cdots$

A MISLEADING PICTURE



III. NUMBER THEORY

1. NORMAL FAMILIES

† High–level languages or computational speed?

• A family of primes $\mathcal{P}$ is *normal* if it contains no primes p, q such that p divides $q-1$.

A: *Three Conjectures*:

◇ *Giuga's conjecture* ('51) is that

$$\boxed{\sum_{k=1}^{n-1} k^{n-1} \equiv n-1 \pmod{n}}$$

if and only if n is prime.

• *Agoh's Conjecture* ('95) is equivalent:

$$\boxed{nB_{n-1} \equiv -1 \pmod{n}}$$

if and only if n is prime; here B_n is a *Bernoulli number*.

◇ *Lehmer's conjecture* ('32) is that

$$\boxed{\phi(n) \mid n-1}$$

if and only if n is prime.

> "A problem as hard as existence of odd perfect numbers."

...

• For these conjectures the set of prime factors of any counterexample n is a normal family.

◇ We exploited this property aggressively in our (Pari/Maple) computations

• Lehmer's conjecture had been variously verified for up to 13 prime factors of n. We extended and <u>unified</u> this for 14 or fewer prime factors.

$\diamond$ We also examined the related condition

$$\boxed{\phi(n) \mid n+1}$$

known to have 8 solutions with up to 6 prime factors (Lehmer) : $2, F_0, \cdots, F_4$ (the *Fermat primes* and a rogue pair: 4919055 and

6992962672132095.

• We extended this to 7 prime factors – by dint of a heap of factorizations!

• But the next Lehmer cases (15 and 8) were way too large. The *curse of exponentiality*!

B. *Counterexamples* to the Giuga conjecture must be *Carmichael numbers**

$$\boxed{(p-1) \mid (\frac{n}{p}-1)}$$

and **odd** *Giuga numbers*: n square-free and

$$\boxed{\sum_{p|n} \frac{1}{p} - \prod_{p|n} \frac{1}{p} \in Z}$$

when $p \mid n$ and p prime. An **even** example is

$$\frac{1}{2}+\frac{1}{3}+\frac{1}{5}-\frac{1}{30}=1.$$

◇ RHS must be '1' for $N < 30$. With 8 primes:

$$554079914617070801288578559178$$

$$= 2 \times 3 \times 11 \times 23\dot{}31 \times 47059$$

$$\times 2259696349 \times 110725121051.$$

† The largest Giuga number we know has 97 digits with 10 primes (one has 35 digits).

*Only recently proven an infinite set!

† Guiga numbers were found by relaxing to a combinatorial problem. We recursively generated *relative primes* forming *Giuga sequences* such as

$$\frac{1}{2}+\frac{1}{3}+\frac{1}{7}+\frac{1}{83}+\frac{1}{5\times 17}-\frac{1}{296310}=1$$

• We tried to 'use up' the only known *branch and bound* algorithm for Giuga's Conjecture: 30 lines of Maple became 2 months in C++ which crashed in Tokyo; but confirmed our local computation that a counterexample n has more than $13,800$ digits.

Coworkers: D. Borwein, P. Borwein, Girgensohn, Wong and Wayne State Undergraduates

2. DISJOINT GENERA

Theorem 1 *There are at most 19 integers not of the form of $xy + yz + xz$ with $x, y, z \geq 1$.*

The only non-square-free are 4 *and* 18. *The first 16 square-free are*

$$1, 2, 6, 10, 22, 30, 42, 58, 70, 78, 102$$

$$130, 190, \mathbf{210}, 330, 462.$$

which correspond to "discriminants with one quadratic form per genus".

• If the 19th exists, it is greater than 10^{11} which the *Generalized Riemann Hypothesis* (GRH) excludes.

• The Matlab road to proof & the hazards of *Sloane's Encyclopedia*.

Coworker: Choi

KUHN

“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.”

HERSH

• Whatever the outcome of these developments, 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 setting:

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

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

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

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

5. Mathematical objects are a special variety of a social-cultural-historical object. Contrary to the assertions of certain 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.

◇ From "Fresh Breezes in the Philosophy of Mathematics", *American Mathematical Monthly*, August-Sept 1995, 589–594.

• The recognition that "quasi-intuitive" analogies may be used to gain insight in mathematics can assist in the learning of mathematics. And honest mathematicians will acknowledge their role in discovery as well.

We should look forward to what the future will bring.

A FEW CONCLUSIONS

- Draw your own! – perhaps $\cdots$

- Proofs are often out of reach – understanding, even certainty, is not.

- Packages can make concepts accessible (Groebner bases).

- Progress is made 'one funeral at a time' (Niels Bohr).

- 'You can't go home again' (Thomas Wolfe).

***

Part I—Mathematics by Experiment:

Plausible Reasoning in the 21st Century

Part II—Experimentation in Mathematics:

Computational Paths to Discovery

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Revised: June 1, 2003

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)

- In his '23' "Mathematische Probleme" lecture to the Paris International Congress, 1900 (see Yandell's, fine account in *The Honors Class*, A.K. Peters, 2002).

IV. ANALYSIS

1. 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 $\mathbf{c_n(t) = m_n(t)/n!}$. 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 $t \geq 1$.

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

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

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

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

(b) As

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

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

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

In particular for $t = 1$, we obtain the sequence

$$1, 1, 2, 4, 9, 21, 51, 127, 323, 835, 2188 \ldots .$$

- These are the *Bell numbers* as was discovered by consulting *Sloane's Encyclopedia*. `www.research.att.com/~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

$$\text{(2)} \qquad \sum_{n\ge 0} c_n u^n = \exp\left(t(e^u - 1)\right).$$

*The Bell numbers were known earlier to Ramanujan – Stigler's Law!

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

Theorem 2 *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 (2) above, we apply this to the sequence $\mathbf{b_j = t/(j-1)!}$ which is log-concave exactly for $t \geq 1$. **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:

$\boxed{\textbf{(??)} \Rightarrow \text{Computer Algebra System} \Rightarrow \text{Interface}}$

$\boxed{\Rightarrow \text{Search Engine} \Rightarrow \text{Digital Library}}$

$\boxed{\Rightarrow \text{Hard New Paper} \Rightarrow \textbf{Answer}}$

- Now if only we could automate this!

2. KHINTCHINE'S CONSTANT

† In different contexts different algorithms star.

A: The celebrated *Khintchine constants* K_0, (K_{-1}) — the limiting geometric (harmonic) mean of the elements of *almost all* simple continued fractions — have efficient reworkings as *Riemann zeta* series.

- ◇ Standard definitions are cumbersome products. $K_0 = 2.6854520010653064453\ldots$

- The rational ζ series we used was:

$$\log(K_0)\ \ln(2)$$

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

Here

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

- When accelerated and used with “recycling” evaluations of $\{\zeta(2s)\}$, this allowed us to compute K_0 to thousands of digits.

- Computation to $7,350$ digits suggests that K_0’s continued fraction obeys its own prediction.

- A related challenge is to find natural constants that provably behave ‘normally’ – in analogy to the *Champernowne* number

$$.0123456789101112\cdots$$

  which is provably normally distributed base ten.

B. *Computing* $\zeta(N)$

$\diamond$ $\boxed{\zeta(2N) \cong B_{2N}}$ can be effectively computed in parallel by

- *multi-section* methods - these have space advantages even as serial algorithms and work for *poly-exp* functions (Kevin Hare);

- FFT–enhanced symbolic *Newton (recycling) methods* on the series $\frac{\sinh}{\cosh}$.

$\diamond$ $\boxed{\zeta(2N+1).}$ The harmonic constant K_{-1} needs odd ζ-values.

• We chose to use identities of Ramanujan et al ...

3. A TASTE of RAMANUJAN

- For $M \equiv -1 \pmod 4$

$$\zeta(4N+3) = -2\sum_{k\geq 1}\frac{1}{k^{4N+3}\left(e^{2\pi k}-1\right)}$$

$$+\frac{2}{\pi}\left\{\frac{4N+7}{4}\zeta(4N+4)-\sum_{k=1}^{N}\zeta(4k)\zeta(4N+4-4k)\right\}$$

where the interesting term is the hyperbolic trig series.

- Correspondingly, for $M \equiv 1 \pmod 4$

$$\zeta(4N+1) = -\frac{2}{N}\sum_{k\geq 1}\frac{(\pi k+N)e^{2\pi k}-N}{k^{4N+1}(e^{2\pi k}-1)^2}$$

$$+\frac{1}{2N\pi}\left\{(2N+1)\zeta(4N+2)+\sum_{k=1}^{2N}(-1)^k 2k\zeta(2k)\zeta(4N+2-2k)\right\}$$

- Only a finite set of $\zeta(2N)$ values is required and the full precision value e^{π} is reused throughout.

◇ The number e^{π} is the easiest transcendental to fast compute (by elliptic methods). One "differentiates" $e^{-s\pi}$ to obtain π (the AGM).

• For $\zeta(4N+1)$ I decoded "nicer" series from a few PSLQ cases of Plouffe. My result is equivalent to:

$$\left\{2-(-4)^{-N}\right\}\sum_{k=1}^{\infty}\frac{\coth(k\pi)}{k^{4N+1}}$$

$$-(-4)^{-2N}\sum_{k=1}^{\infty}\frac{\tanh(k\pi)}{k^{4N+1}}$$

$$=Q_N\times\pi^{4N+1}. \tag{3}$$

The quantity Q_N in (3) 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

$$\coth(x) = 1 + \frac{2}{\exp(2x)-1}$$

one may solve for

$$\zeta(4N+1).$$

• Thus,

$$\zeta(5) = \frac{\mathbf{1}}{\mathbf{294}}\pi^{\mathbf{5}} + \frac{2}{35}\sum_{k=1}^{\infty}\frac{1}{(1+e^{2k\pi})k^5}$$

$$+\frac{72}{35}\sum_{k=1}^{\infty}\frac{1}{(1-e^{2k\pi})k^5}.$$

- Will we ever be able to identify universal formulae like (4) automatically? My solution was highly human assisted.

Coworkers: Bailey, Crandall, Hare, Plouffe.

V: INTEGER RELATION EXAMPLES

1. The USES of LLL and PSLQ

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

$$\boxed{0 = a_1 x_1 + a_2 x_2 + \cdots + a_n x_n.}$$

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.

- $(n \geq 3)$ 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

$$\begin{aligned} S_2 := \zeta(2) &= 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k}} \\ A_3 := \zeta(3) &= \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^3 \binom{2k}{k}} \\ S_4 := \zeta(4) &= \frac{36}{17} \sum_{k=1}^{\infty} \frac{1}{k^4 \binom{2k}{k}} \end{aligned}$$

◇ These results might suggest that

$$Z_5 \;:=\; \zeta(5) / \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^5 \binom{2k}{k}}$$

is a simple rational or algebraic number.
PSLQ RESULT: If Z_5 satisfies a polynomial of degree ≤ 25 the Euclidean norm of coefficients *exceeds* 2×10^{37}.

2. BINOMIAL SUMS and LIN_DEP

• 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” showed).

• But ⋯ PSLQ yields in *polylogarithms*:

$$\begin{aligned} A_5 &= \sum_{\mathbf{k}=1}^{\infty} \frac{(-1)^{\mathbf{k}+1}}{\mathbf{k}^5 \binom{2\mathbf{k}}{\mathbf{k}}} = 2\zeta(5) \\ &- \tfrac{4}{3}L^5 + \tfrac{8}{3}L^3\zeta(2) + 4L^2\zeta(3) \\ &+ 80 \sum_{n>0} \left(\frac{1}{(2n)^5} - \frac{L}{(2n)^4} \right) \rho^{2n} \end{aligned}$$

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 $\zeta(7), \zeta(9), \zeta(11)\ldots$.

◇ 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:

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

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

Theorem 3 *For any complex z,*

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

$$(5) \quad = \sum_{k=1}^{\infty} \frac{1}{k^3(1 - z^4/k^4)}$$

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

◇ The first '=' is easy. The second is quite unexpected in its form!

• $z = 0$ yields Apéry's formula for $\zeta(3)$ and the coefficient of z^4 is (4).

HOW IT WAS FOUND

◇ The first ten cases show (5) has the form

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

for undetermined P_k; with abundant data to compute

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

• We found many reformulations of (5), including a marvellous finite sum:

$$\boxed{\sum_{k=1}^{n}\frac{2n^2}{k^2}\frac{\prod_{i=1}^{n-1}(4k^4+i^4)}{\prod_{i=1,\, i\neq k}^{n}(k^4-i^4)}=\binom{2n}{n}.} \tag{6}$$

◇ Obtained via Gosper's (Wilf-Zeilberger type) *telescoping algorithm* after a mistake in an electronic Petrie dish ('infty' $\neq$ 'infinity').

This identity was subsequently proved by Almkvist and Granville (Experimental Math, 1999) thus finishing the proof of (5) and giving a rapidly converging series for any $\zeta(4N+3)$ where N is positive integer.

$\diamond$ 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).

† Paul Erdos, when shown (6) 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 ('$\zeta(3)$ is irrational').

3. MULTIPLE ZETA VALUES & LIN_DEP

• *Euler sums* or *MZVs* ("multiple zeta values") are a wonderful generalization of the classical ζ function.

• For natural numbers $i_1, i_2, \ldots, i_k$

$$\zeta(i_1, i_2, \ldots, i_k) := \sum_{n_1 > n_2 > \dot{n}_k > 0} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}} \tag{7}$$

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

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

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

  - Definition (7) clearly extends to alternating and character sums. MZVs have recently found interesting interpretations in high energy physics, knot theory, combinatorics ...

- MZVs satisfy many striking identities, of which

$$\zeta(2,1) = \zeta(3)$$

$$4\zeta(3,1) = \zeta(4)$$

are the simplest.

  ◇ Euler himself found and partially proved theorems on reducibility of depth 2 to depth 1 ζ's [$\zeta(6,2)$ is the lowest weight 'irreducible].

◇ High precision *fast* ζ-*convolution* (EZFace/Java) allows use of integer relation methods and leads to important dimensional (reducibility) conjectures and amazing identities.

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

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

- Series converge absolutely for $|x| < 1$ (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 equations**

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

if $n_r \geq 2$ 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 $\overline{s} := (s_1, s_2, \ldots, s_N)$. 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 $\mathbf{D_s F = t^s F}$ 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:

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

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

B. Similarly, for $N = 1$ and negative integers

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

and $L_{\overline{-1}}(2x-1,t)$ 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

$$\begin{aligned}
t^6\, F &= x^2(x-1)^2(x+1)^2\, D^6 F \\
&+ x(x-1)(x+1)(15x^2-6x-7)\, D^5 F \\
&+ (x-1)(65x^3+14x^2-41x-8)\, D^4 F \\
&+ (x-1)(90x^2-11x-27)\, D^3 F \\
&+ (x-1)(31x-10)\, D^2 F + (x-1)\, DF.
\end{aligned}$$

- 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 4 (BBGL) *For $|x|, |t| < 1$ and integer $n \geq 1$*

$$\begin{aligned} \sum_{n=0}^{\infty} & \quad L(\underbrace{3,1,3,1,\ldots,3,1}_{n-fold};x)\,t^{4n} \\ = & \quad F\left(\frac{t(1+i)}{2}, \frac{-t(1+i)}{2};1;x\right) \\ \times & \quad F\left(\frac{t(1-i)}{2}, \frac{-t(1-i)}{2};1;x\right). \end{aligned} \tag{8}$$

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

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

QED

- 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 5 *(**Zagier Conjecture**)*

$$\zeta(\underbrace{3,1,3,1,\ldots,3,1}_{n-fold}) = \frac{2\,\pi^{4n}}{(4n+2)!} \tag{9}$$

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 (8) 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 (8) ends the proof. **QED**

- What other deep Clausen-like hypergeometric factorizations lurk within?

- If one suspects that (5) 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 $\zeta(2n)$.

A striking conjecture (open for $n > 2$) is:

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

or equivalently that the functions

$$L_{-2,1}(1,2t) = L_{2,1}(1,t) \qquad (= L_3(1,t)),$$

agree for small t. There is abundant evidence amassed since it was found in 1996.

- This is the only identification of its type of an Euler sum with a distinct MZV . Can just $n = 2$ be proven symbolically as is the case for $n = 1$?

DIMENSIONAL CONJECTURES

- To sum up, our simplest conjectures (on the number of irreducibles) are still beyond present proof techniques. Does $\zeta(5)$ or $G \in \mathbb{Q}$? This may or may not be close to proof! Thus, the field is wide open for numerical exploration.

- Dimensional conjectures sometimes involve finding integer relations between hundreds of quantities and so demanding precision of thousands of digits – often of hard to compute objects.

- In that vein, Bailey and Broadhurst have recently found a *polylogarithmic ladder* of length 17 (a record) with such "ultra-PSLQing".

A conjectured generating function for the *dimension* of a *minimal generating set* of the $(\mathbf{Q}, +, \cdot)$-algebra containing all Euler sums of weight n and depth k, $E_{n,k}$.

$$\prod_{n\geq 3}\prod_{k\geq 1}\left(1-x^n y^k\right)^{E_{n,k}} \stackrel{?}{=} 1-\frac{x^3 y}{(1-x^2)(1-xy)}$$

- Over 18 months of computation provided the results in the next table and were very convincing. As it was for a generating function which would prove more than:

  Conjecture. (Drinfeld(1991)-Deligne) The graded Lie algebra of *Grothendieck & Teichmuller* has no more than one generator in odd degrees, and no generators in even degrees.

$E_{n,k}$ n k	1	2	3	4	5	6
3	1					
4		1				
5	1		1			
6		1		1		
7	1		2		1	
8		2		2		1
9	1		3		3	
10		2		5		3
11	1		5		7	
12		3		8		9
13	1		7		14	
14		3		14		20
15	1		9		25	
16		4		20		42
17	1		12		42	
18		4		30		75
19	1		15		66	
20		5		40		132

Coworkers: B^4, Fee, Girgensohn, Lisoněk, others.

4. MULTIPLE CLAUSEN VALUES

We also studied *Deligne words* for integrals generating *Multiple Clausen Values* at $\frac{\pi}{3}$ like

$$\mu(a,b) := \sum_{n>m>0} \frac{\sin(n\frac{\pi}{3})}{n^a m^b},$$

and which seem quite fundamental.

• Thanks to a note from Flajolet, which led to proof of results like $S_3 = \frac{2\pi}{3}\mu(2) - \frac{4}{3}\zeta(3)$,

$$\sum_{k=1}^{\infty} \frac{1}{k^5 \binom{2k}{k}} = 2\pi\mu(4) - \frac{19}{3}\zeta(5) + \frac{2}{3}\zeta(2)\zeta(3),$$

$$\sum_{k=1}^{\infty} \frac{1}{k^6 \binom{2k}{k}} = -\frac{4\pi}{3}\mu(4,1) + \frac{3341}{1296}\zeta(6) - \frac{4}{3}\zeta(3)^2.$$

I finish with another sort of extension:

$$\sum_{n=1}^{\infty} \frac{1}{n^3 \binom{3\,n}{n} 2^n} = \frac{1}{6} \ln^3(2) - \frac{33}{16} \zeta(3) - \frac{1}{24} \pi^2 \ln(2) + \pi\, G.$$

Coworkers: Broadhurst & Kamnitzer

CARATHÉODORY

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

- Constantin Carathéodory, speaking to an MAA meeting in 1936.

GAUSS

- In Boris Stoicheff's enthralling biography of Gerhard Herzberg (1903-1999), who fled Germany for Saskatchewan in 1935 and won the 1971 Nobel Prize in Chemistry, Gauss is recorded as writing:

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

- **Nationally shared —— Internationally competitive**

  The scope of the C3.ca is a seven year plan to build computational infrastructure on a scale that is globally competitive, and that supports globally competitive research and development. The plan will have a dramatic impact on Canada's ability to develop a knowledge based economy. It will attract highly skilled people to new jobs in key application areas in the business, research, health, education and telecommunications sectors. It will provide the tools and opportunity to enhance their knowledge and experience and retain this resource within the country.

- The Canadian government has funded/matched $200 million worth of equipment in the last three years.

  - Ten major installations in Five Provinces.

  - More to come: long-term commitment?

  - Good human support at a distance/web collaboration and visualization tools are key.

  - A pretty large, and successful, investment for a medium size country.

  - A good model for other such countries?

- `www.westgrid.ca` and `www.colab.sfu.ca` are the projects I am directly involved in.

How not to experiment

Pooh Math:
'Guess and Check'
while
Aiming Too High

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*Quotations are at `jborwein/quotations.html`