Experimental Mathematics

and

Exact Computation

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ABSTRACT. My intention is to discuss experimental computation from a mathematician's perspective. Using, for the most part, various of the zeta functions and related polylogarithmic functions with which I have worked I shall try to illustrate what is currently easy, what is hard, what is possible and what we aspire to be be able to do.

I shall discuss a few of the underlying philosophical issues and shall also summarize some of the very demanding exact (symbolic/numeric) computations I have undertaken in the last few years with David Bailey, David Bradley, David Broadhurst, Petr Lisoněk, Peter Borwein and others.

HADAMARD

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

◇ Quoted in E. Borel, *Lecons sur la theorie des fonctions*, 1928

MOTIVATION

GOAL is INSIGHT – demands speed ≡ 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 ≡ more space, speed & stuff.
- Exact ≡ hybrid ≡ symbolic '+' numeric.
- 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
- Do what is easy for the computer (and what is possible).

PART of OUR 'METHODOLOGY'

1. (*High Precision*) computation of object(s).
2. *Pattern Recognition* of *real numbers* (Inverse Calculator)*. or *sequences* (Salvy & Zimmermann's 'gfun', Sloane's Encyclopedia)
3. Extensive use of 'Integer Relation Methods': *PSLQ* & *LLL*.
   - Exclusion bounds are especially useful.
   - Great test bed for "Experimental Mathematics".
4. Some automated theorem proving (Wilf-Zeilberger etc.).

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

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 **Galilean**: "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*

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."

• But Symbols are more reliable than pictures.On to the examples ...

I: WARM-UP EXAMPLES

1. TWO INTEGRALS

• A. $\pi \neq \frac{22}{7}$.

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

...

• *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*:

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

...

• *B. and a transcendent one*:

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

3. HIGH PRECISION FRAUD

and CONTINUED FRACTIONS

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

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

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

4. PARTIAL FRACTIONS & CONVEXITY

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

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

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

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

⋄ For $N = 3$ there are 6 permutations of

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

• 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:

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

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

CONJECTURE. For each $N \in \mathbb{N}$ the function $p_N : \mathbb{R}_+^N \to \mathbb{R}_+$ by

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

is convex. For $N < 5$ a large symbolic Hessian computation proves this.

† Is $N = 5$ provable symbolically? [Details in *SIAM Electronic Problems*.]

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."

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). His present world record is 2^{36} digits in April 1999.

⋄ 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<u>2</u> ! And after 18 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.

⋄ Set

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

and iterate

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

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.

⋄ Once found, easy to prove in Mathematica, Maple or by hand.

◇ 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

$$\underline{0}0000111110011111.$$

• The quadrillionth bit is coming $\cdots$

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

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

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

• Why was G missed earlier?

• He also gives some constants with ternary expansions.

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

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 unified this for 14 or fewer prime factors.

◇ 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:

$$5540799146170708012885785591 78$$

$$= 2 \times 3 \times 11 \times 23\dot{3}1 \times 47059$$

$$\times 2259696349 \times 110725121051.$$

† 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. 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

3. 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.

• The rational ζ series we used was:

$$\ln K_0 \ln 2 = \sum_{n=1}^{\infty} \frac{\zeta(2n) - 1}{n} \left(1 - \frac{1}{2} + \frac{1}{3} - \ldots + \frac{1}{2n-1}\right).$$

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* $\zeta(N)$

⋄ $\boxed{\zeta(2N) \cong B_{2N}}$ 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 $\frac{\sinh}{\cosh}$.

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

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

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've lately decoded "nicer" series from a few PSLQ cases of Plouffe. It is equivalent to:

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

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

(1) $$= Q_N \times \pi^{4N+1}.$$

⋄ The quantity Q_N in (1) is an explicit rational:

(2) $$Q_N := \sum_{k=0}^{2N+1}\frac{B_{4N+2-2k}B_{2k}}{(4N+2-2k)!(2k)!} \times \left\{(-1)^{\binom{k}{2}}(-4)^N 2^k + (-4)^k\right\}.$$

- 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,

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

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

⋄ Will we ever be able to identify universal formulae like (2) automatically? My solution was highly human assisted.

Coworkers: Bailey, Crandall, Hare, Plouffe.

IV: 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).

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.

ZETA FUNCTIONS

• Recall that the *zeta function* is defined by

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

for $s > 1$.

• 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 suggest

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

might be 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 $\cdots$ PSLQ yields in *polylogarithms*:

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

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:

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

• 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. For any complex z,

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

⋄ 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 (3).

HOW IT WAS FOUND

⋄ The first ten cases show (4) 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 (4), including a marvelous finite sum:

$$(5) \quad \boxed{\sum_{k=1}^{n}\frac{2n^2}{k^2}\frac{\prod_{i=1}^{n-1}(4k^4+i^4)}{\prod_{i=1,\, i\neq k}^{n}(k^4-i^4)} = \binom{2n}{n}.}$$

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

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

⋄ And perhaps shedding light on the irrationality of $\zeta(7)$? Recall that $\zeta(2N+1)$ is not proven irrational for $N > 1$.

† Paul Erdos, when shown (5) 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 and LIN_DEP

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

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

$$\zeta(i_1, i_2, \ldots, i_k) := \sum_{n_1>n_2>\cdots>n_k>0} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}} \tag{6}$$

⋄ 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 (6) 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').

⋄ A high precision *fast ζ-convolution* (EZFace/Java) allows use of integer relation algorithms leading to important dimensional (reducibility) conjectures and amazing identities.

• We illustrate with a conjecture of Zagier first proved by Broadhurst et al:

$$\zeta(\{3,1\}_n) = \frac{1}{2n+1}\zeta(\{2\}_{2n}) \quad \left(= \frac{2\pi^{4n}}{(4n+2)!}\right) \tag{7}$$

where $\{s\}_n$ is the string s repeated n times.

† The *unique* non-commutative analogue of Euler's evaluation of $\zeta(2n)$.

⋄ My favourite conjecture (open for $n > 2$) is

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

Can just $n = 2$ be proven symbolically as is the case for $n = 1$?

• Our simplest conjectures (on the number of irreducibles) are beyond present proof techniques. Does $\zeta(5)$ or $G \in \mathbb{Q}$?

⋄ 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.

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

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

4. MULTIPLE CLAUSEN VALUES

• We are now studying *Deligne words* for multiple integrals generating *Multiple Clausen Values* at $\pi/3$ such as

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

and which seem quite fundamental.

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

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

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

Coworkers: Broadhurst & Kamnitzer

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."

A FEW CONCLUSIONS

- Draw your own! – perhaps ···
- 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).

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◇ Quotations at jborwein/quotations.html