Numerical and computational mathematics

(at the undergraduate level)

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RATIONALE

- towards an Experimental Mathodology – philosophy and practice

- intutition is acquired – teach computation and mathematics together

- "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

- learn what is easy for the computer (and what is possible)

- marriage of research, teaching, applications ("life long learning" etc)

BOTTLENECKS

- level of classroom technology
- skill set of faculty (and students)
- conservatism of faculty
- need for ease of use – analogies with texts
- time available in class
- preparation time available

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."

I: FAIRLY ELEMENTARY EXAMPLES

1. EVALUATING two INTEGRALS

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

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

$$\cdots$$

- *B. The sophomore's dream.*

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

2. EVALUATING some 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. 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.

4. 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 to 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

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

5. PARTIAL FRACTIONS and 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 $n = 3$ this is

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

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

• 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 **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.

• Check $N < 5$ via large symbolic Hessian. **PROOF.** A year later, *joint expectations* gave:

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

[See *SIAM Electronic Problems and Solutions*.]

6a. DRAWING CONVEX CONES

QUESTION: Can one construct a convex compact set P in $\mathbb{R}^3$ that fails to be polyhedral at exactly one point?

• That depends on the precise 'definitions' ...

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6b. DRAWING GRADIENT FIELD RANGES

QUESTION: Suppose $b : \mathbb{R}^2 \to \mathbb{R}^+$ is C^1 and has support in the unit circle? What can one say about the range of ∇b?

• $0 \in \operatorname{int} R(\nabla b)$ is connected but $R(\nabla b)$ need not be convex or simply connected.

† Much more I do not know.

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: LESS ELEMENTARY EXAMPLES

7. The USES of LLL

and INTEGER RELATION DETECTION

• 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

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

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

If α is computed to high precision apply LLL to the vector

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

- Solution integers a_i are coefficients of a polynomial 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

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

◇ 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}.

8. 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*:

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

where $L := \log(\rho)$ and $\rho := (\sqrt{5}-1)/2$; with similar formulae for A_4, A_6.

• 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:

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

• 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,

$$\sum_{n=1}^{\infty} \zeta(4n+3) z^{4n}$$

$$(2) \qquad = \sum_{k=1}^{\infty} \frac{1}{k^3(1 - z^4/k^4)}$$

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

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

• $z = 0$ yields Apéry's formula for $z(3)$ and the coefficient of z^4 is (1).

HOW IT WAS FOUND

⋄ The first ten cases show (2) has the form

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

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 (2), including a marvellous finite sum:

$$\text{(3)}\quad \boxed{\sum_{k=1}^{n}\frac{2n^2}{k^2}\frac{\prod_{i=1}^{n-1}(4k^4+i^4)}{\prod_{i=1,\, i\neq k}^{n}(k^4-i^4)}=\binom{2n}{n}.}$$

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

• This identity was recently proved by Almkvist and Granville, thus finishing the proof of (2) 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 (3) 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').

9. MINIMAL POLYNOMIALS of 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

$$\begin{aligned} A^2 &= C^2 = I \\ B^2 &= CA, AC = B. \end{aligned} \tag{4}$$

• 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 (4)

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

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

• The truth is I started with instances of

$$`minpoly(M, x)'$$

and then emboldened I typed

$$`minpoly(B, x)'$$

in Maple ...!

• Random matrices have full degree *minimal polynomials*.

† *Jordan Forms* uncover Spectral Abscissas.

10. PARTITIONS and PATTERNS

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

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

⋄ 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), an d 2000 (for Maple)?

...

• *Euler's pentagonal number theorem* is

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

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

11. 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 $i_1, i_2, \ldots, i_k$

$$\zeta(i_1, i_2, \ldots, i_k) := \sum_{n_1 > n_2 > n_k > 0} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}} \tag{5}$$

◇ 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 (5) clearly extends to alternating 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) 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:

$$\zeta(\{3,1\}_n) = \frac{1}{2n+1}\zeta(\{2\}_{2n})$$
$$\left(= \frac{2\pi^{4n}}{(4n+2)!}\right) \qquad (6)$$

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

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

◇ My favourite open conjecture ($n > 2$) is

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

Can $n = 2$ be proven symbolically?

• Our simplest dimensional conjectures are beyond present proof techniques. Does $\zeta(5) \in Q$?

12. The USE of the GFUN PACKAGE

• Sloane's Encyclopedia allows one to look up sequences like

$$1, 3, 5, 11, 15, 21, 29, 35, 39, 51, 65, 95, 105, 165, 231$$

and our *Inverse Symbolic Calculator* allows one to look up floating point numbers:

⋄ For example, 1.2720196495 will be identified as

$$\sqrt{\frac{\sqrt{5}+1}{2}}$$

by the ISC (or by LLL).

• Salvy and Zimmerman's *GFUN* package allows one to guess *generating functions* and manipulate them:

⋄ For example, what is the next term in the sequence

$$1, 1, 4, 9, 25, 64, 169, 441\,?$$

13. KARATSUBA MULTIPLICATION

• The only arithmetic operation we perform optimally is $\pm$. We know very little about *optimal methods* for computations such as (matrix) multiplication or π and γ.

$\diamond$ But we can teach about *complexity*, the *Fast Fourier Transform* and many other neat things.

• Karatsuba's fundamental observation was that:

$$\begin{array}{rcl} (a + b\,10^n) & \times & (c + d\,10^n) \\ & = & \\ \underbrace{a \times c} & + & \underbrace{b \times d}\,10^{2n} \\ & + & \\ \{\underbrace{(a+b)\times(c+d)} & - & \underbrace{(ac+bd)}_{\text{KNOWN}}\}\,10^n \end{array}$$

• This replaces 2 multiplications of length $2n$ by 3 of length n and so effective reduces the work in multiplication from growing asymptotically like n^2 to $n^{\log_2(3)}$.

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."

CONCLUSIONS

- Draw your own! – perhaps ...
- Computing can animate teaching
- Packages can make concepts accessible (Groebner bases)
- Technology can enhance understanding and add relevance
- Progress is made ‘one funeral at a time’ (Niels Bohr)
- ’You can’t go home again’ (Thomas Wolfe)

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One REFERENCE

J. Borwein & R. Corless, "Emerging Tools for Experimental Mathematics," *MAA Monthly*, **106** (1999), 889–909.

† Available as CECM Preprint 98:110.

⋄ Quotations at jborwein/quotations.html