The Experimental Mathematician:

A Computational Guide

to the Mathematical Unknown

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1

EINSTEIN'S SAVAGE CERTAINTY



2

ABSTRACT I speak primarily from the perspective of an informed consumer, and only secondarily as a producer of, mathematical software (www.mathresources.com).

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, 3, 7].

*For example, WestGrid, the new Western Canadian computer grid (www.westgrid.ca), and my own advanced collaboration facility, CoLab (www.colab.sfu.ca).

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 ([6-8]) such as:

QUESTIONS

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? ('embodied cognition')
- Who cares for certainty? What is the role of proof?
- And I shall offer some personal conclusions from a *subset* of these overheads.

5

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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."*

*'23' Mathematische Probleme' lecture to the Paris International Congress, 1900 (Yandell, *The Honors Class*).

6

 References are available at http://www.cecm.sfu.ca/preprints/

The transparencies, and other resources, for this and related presentations are lodged at www.cecm.sfu.ca/personal/jborwein/cmesg25.html

A companion paper is

7. J. M. Borwein, "The Experimental Mathematician: The Pleasure of Discovery and the Role of Proof," *International Journal of Computers for Mathematical Learning*, in press, 2002. [CECM Preprint 02:178].

and a forthcoming book is

8. D.H. Bailey, J.M. Borwein, R Girgensohn (and K. Devlin), "The Experimental Mathematician: A Computational Guide to the Mathematical Unknown", A.K. Peters Ltd. (In preparation, 2002) ISBN: 1-56881-136-5.

BRIGGS

'... where almost one quarter hour was spent, each beholding the other with admiration before one word was spoken: at last Mr. Briggs began "My Lord, I have undertaken this long journey purposely to see your person, and to know by what wit or ingenuity you first came to think of this most excellent help unto Astronomy, viz. the Logarithms: but my Lord, being by you found out, I wonder nobody else found it out before, when now being known it appears so easy." "*

*Henry Briggs is describing his first meeting in 1617 with Napier whom he had traveled from London to Edinburgh to meet. Quoted from H.W. Turnbull's *The Great Mathematicians*, Methuen, 1929.

• Many of my favourite 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].

They rely on the use of *Integer Relations Algorithms* — recently ranked among the 'top ten' algorithms of the century [5, 6]. See [3,4] and www.cecm.sfu.ca/projects/IntegerRelations/



10

INTRODUCTION

Ten years ago I was offered the signal opportunity to found the Centre for Experimental and Constructive Mathematics (CECM) at Simon Fraser. On our web-site (www.cecm.sfu.ca) I wrote:

"At CECM we are interested in developing methods for exploiting mathematical computation as a tool in the development of mathematical intuition, in hypotheses building, in the generation of symbolically assisted proofs, and in the construction of a flexible computer environment in which researchers and research students can undertake such research. That is, in doing 'Experimental Mathematics.'"

CECM

The decision to build CECM was based:

- (i) on more than a decade's personal experience, largely since the advent of the personal computer, of the value of computing as an adjunct to mathematical insight and correctness;
- (ii) on a growing conviction that the future of mathematics would rely much more on collaboration and intelligent computation;
- (iii) on the premise that such developments needed to be enshrined in, and were equally valuable for, mathematical education; and
- (iv) on the premise that experimental mathematics is *fun*.

TEN YEARS LATER

Ten years later, my colleagues and I are even more convinced of the value of our venture — and the 'mathematical universe is unfolding' much as we anticipated. Our efforts and philosophy are described in some detail in the forthcoming book and in the survey articles [1,3,4,6]. More technical accounts of some of our tools and successes are detailed in [2].

⋄ Ten years ago the term 'experimental mathematics' was often treated as an oxymoron. Now there is a highly visible and high quality journal of the same name.

AND FIFTEEN YEARS AGO

Fifteen years ago, most self respecting research pure mathematicians would not admit to using computers as an adjunct to research. Now they will talk about the topic whether or not they have any expertise.

The centrality of information technology to our era and the growing need for concrete implementable answers suggests why we have attached the word 'Constructive' to CECM.

13

PLUS ÇA CHANGE

While some things have happened much more slowly than we guessed (e.g., good character recognition (OCR) for mathematics, any substantial impact on classroom parole) others have happened much more rapidly (e.g., the explosion of the world wide web*, the quality of graphics and animations, the speed and power of computers).

• Crudely, the tools with broad societal or economic value arrive rapidly, those interesting primarily in our niche do not.

Research mathematicians for the most part neither think deeply about nor are terribly concerned with either pedagogy or the philosophy of mathematics.

*Our web site now averages well over a million accesses a month

15

THE AESTHETIC IMPULSE

Nonetheless, aesthetic and philosophical notions have always permeated (pure and applied) mathematics. And the top researchers have always been driven by an aesthetic imperative*:

^{*}Quoted by Ram Murty in *Mathematical Conversations, Selections from The Mathematical Intelligencer*, compiled by Robin Wilson and Jeremy Gray, Springer-Verlag, New York, 2000.

ARTIN

"We all believe that mathematics is an art. The author of a book, the lecturer in a classroom tries to convey the structural beauty of mathematics to his readers, to his listeners. In this attempt, he must always fail. Mathematics is logical to be sure, each conclusion is drawn from previously derived statements. Yet the whole of it, the real piece of art, is not linear; worse than that, its perception should be instantaneous. We have all experienced on some rare occasions the feeling of elation in realizing that we have enabled our listeners to see at a moment's glance the whole architecture and all its ramifications."

17

19

(Emil Artin, 1898-1962)

AESTHETICS & UTILITY

Elsewhere, I have similarly argued for aesthetics before utility.* The opportunities to tie research and teaching to aesthetics are almost boundless — at all levels of the curriculum.†

This is in part due to the increasing power and sophistication of visualization, geometry, algebra and other mathematical software.

- That said, in my online lectures and resources and in many of the references one will find numerous examples of the utility of experimental mathematics such as *gravitational boosting*.
- *J. M. Borwein, "Aesthetics for the Working Mathematician," in *Beauty and the Mathematical Beast*, in press (2002). [CECM Preprint 01:165].
- [†]An excellent middle school illustration is described in Nathalie Sinclair, "The aesthetics is relevant," for the learning of mathematics, **21** (2001), 25-32.

18

MY PRESENT AIM

In this setting, my primary concern is to explore the relationship between proof (deduction) and experiment (induction). I shall borrow shamelessly from my earlier writings.

There is a disconcerting pressure at all levels of the curriculum to derogate the role of proof.

This is in part motivated by the aridity of some traditional teaching (e.g., Euclid), by the alternatives offered by good software, by the difficulty of teaching and learning the tools of the traditional trade, and perhaps by laziness.

My own attitude is perhaps best summed up by a cartoon in a book on learning to program in APL (a very high level language).

The blurb above reads:

"Remember ten minutes of computation is worth ten hours of thought."

The blurb below reads:

"Remember ten minutes of thought is worth ten hours of computation."

Just as 'the unlived life is not much worth examining' (Charles Krauthammer, et al), proof and rigour should be in the service of things worth proving.

• And equally foolish, but pervasive, is encouraging students to 'discover' fatuous generalizations of uninteresting facts.

GAUSS, HADAMARD & HARDY (GHH)

Three of my personal mathematical heroes, very different men from different times, all testify interestingly on these points and on the nature of mathematics.

21

He was right, as it pried open the whole vista of nineteenth century elliptic and modular function theory. Gauss's specific discovery, based on tables of integrals provided by Stirling (1692-1770), was that the reciprocal of the integral

$$\frac{2}{\pi} \int_0^1 \frac{dt}{\sqrt{1 - t^4}}$$

agreed numerically with the limit of the rapidly convergent iteration given by $a_0:=1,\ b_0:=\sqrt{2}$ and computing

$$a_{n+1} := \frac{a_n + b_n}{2}, \quad b_{n+1} := \sqrt{a_n b_n}$$

The sequences a_n, b_n have a common limit 1.1981402347355922074...

• Which object, the integral or the iteration, is more familiar, which is more elegant — then and now?

GAUSS

Carl Friedrich Gauss (1777-1855) wrote*

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

One of Gauss's greatest discoveries, in 1799, was the link between the <u>lemniscate sine</u> function and the <u>arithmetic-geometric mean</u> iteration.

This was based on a purely computational observation. The young Gauss wrote in his diary that the result

"will surely open up a whole new field of analysis."

*See "Isaac Asimov's Book of Science and Nature Quotations," Weidenfield and Nicolson, New York (1988).

22

··· CRITERIA CHANGE

'Closed forms' have yielded centre stage to 'recursion', much as biological and computational metaphors (even 'biology envy') have replaced Newtonian mental images with Richard Dawkin's 'blind watchmaker'.

This experience of 'having the result' is reflective of much research mathematics. Proof and rigour play the role described next by Hadamard.

- Likewise, the back-handed complement given by Briggs to Napier underscores that is often harder to discover than to explain or digest the new discovery.
- ⋄ "Hardy asked 'What's your father doing these days. How about that esthetic measure of his?' I replied that my father's book was out. He said, 'Good, now he can get back to real mathematics'." (Garret Birkhoff).

HADAMARD

A constructivist, experimental and aesthetic driven rationale for mathematics could hardly do better than to start with:

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*)

Jacques Hadamard (1865-1963) was perhaps the greatest mathematician to think deeply and seriously about cognition in mathematics[†].

*In E. Borel, "Lecons sur la theorie des fonctions," 1928, quoted by George Polya in *Mathematical discovery: On understanding, learning, and teaching problem solving* (Combined Edition), New York, John Wiley (1981), pp. 2-126.

†Other than Poincaré?

25

Hadamard is quoted as saying "... in arithmetic, until the seventh grade, I was last or nearly last" which should give encouragement to many young students.

Hadamard was both the author of "The psychology of invention in the mathematical field" (1945), a book still worth close inspection, and co-prover of the <u>Prime Number Theorem</u> (1896):

"The number of primes less than n tends to ∞ as does $\frac{n}{\log n}$."

This was one of the culminating results of 19th century mathematics and one that relied on much preliminary computation and experimentation.

26

IN PART BECAUSE

One rationale for experimental mathematics and for heuristic computations is that one generally does not know during the course of research how it will pan out. Nonetheless, one must frequently prove all the pieces along the way as assurance that the project remains on course.

• The methods of experimental mathematics, alluded to below, allow one to maintain the necessary level of assurance without nailing down all the lemmas.

At the end of the day, one can decide if the result merits proof. It may not it may not be the answer one sought, or it just may not be interesting enough.

HARDY'S APOLOGY

Correspondingly, G. H. Hardy (1877-1947), the leading British analyst of the first half of the twentieth century was also a stylish author who wrote compellingly in defense of pure mathematics.

In his apologia, "A Mathematician's Apology" * Hardy writes

"All physicists and a good many quite respectable mathematicians are contemptuous about proof."

The Apology is a spirited defense of beauty over utility:

"Beauty is the first test. There is no permanent place in the world for ugly mathematics."

*The Apology is one of Amazon's best sellers.

That said, his comment that

"Real mathematics . . . is almost wholly 'useless'."

has been over-played and is now to my mind very dated, given the importance of cryptography and other pieces of algebra and number theory devolving from very pure study. But he does acknowledge that

"If the theory of numbers could be employed for any practical and obviously honourable purpose, ..."

even Gauss would be persuaded.

• The existence of Amazon, or Google, means that I can be less than thorough with my bibliographic details without derailing anyone who wishes to find the source.

29

THE LIMITS OF REASON

Such examples show forcibly the limits on experimentation, at least of a naive variety.

Many will be familiar with the 'Law of large numbers' in statistics. Here we see what some number theorists call the 'Law of small numbers': all small numbers are special, many are primes and direct experience is a poor guide.

And sadly or happily depending on one's attitude even 10^{1166} may be a small number. In more generality one never knows when the initial cases of a seemingly rock solid pattern are misleading.

• Consider the classic sequence counting the maximal number of regions obtained by joining n points around a circle by straight lines:

$$1, 2, 4, 8, 16, 31, 57, \cdots$$

(Entry A000127 in Sloane's Encyclopedia.)

A STRIKING EXAMPLE

Hardy, on page 15 of his tribute to Ramanujan entitled *Ramanujan*, *Twelve Lectures* ..., gives the so-called 'Skewes number' as a "striking example of a false conjecture".

The integral

$$\operatorname{li} x = \int_0^x \frac{dt}{\log t}$$

is a very good approximation to $\pi(x)$, the number of primes not exceeding x. Thus, li $10^8 = 5,762,209.375...$, while $\pi(10^8) = 5,761,455$.

It was conjectured that

$$li x > \pi(x)$$

holds for all x and indeed it is so for many x. Skewes in 1933 showed the first explicit crossing at $10^{10^{10^{34}}}$.

 \bullet This is now reduced to a tiny number, a mere 10^{1167} , still vastly beyond direct computational reach or even insight.

30

MY OWN METHODOLOGY

As a computational and experimental pure mathematician my main goal is: *insight*. Insight demands speed and increasingly parallelism as described in [6].

Extraordinary speed and enough space are prerequisite for rapid verification and for validation and falsification ('proofs and refutations'.) One can not have an 'aha' when the 'a' and 'ha' come minutes or hours apart.

• What is 'easy' changes as computers and mathematical software grow more powerful. We see an exciting merging of disciplines, levels and collaborators.

We are more and more able to: marry theory & practice, history & philosophy, proofs & experiments; to match elegance and balance to utility and economy; and to inform all mathematical modalities computationally: analytic, algebraic, geometric & topological.

This has lead us to articulate an *Experimental Mathodology*, as a philosophy [1] and in practice [3], based on:

- (i) meshing computation and mathematics (intuition is acquired not natural) "gravitational boosting");
- (ii) visualization (even three is a lot of dimensions). Nowadays we can exploit pictures, animations, emersive reality (e.g. KnotPlot), sounds and other haptic stimuli; and on
- (iii) 'caging' and 'monster-barring' (Imre Lakatos's terms for how one rules out exceptions and refines hypotheses).

Two particularly useful components are:

- graphic checks: comparing $2\sqrt{y} y$ and $\sqrt{y} \ln(y)$, 0 < y < 1 pictorially is a much more rapid way to divine which is larger that traditional analytic methods.
- randomized checks: of equations, linear algebra, or primality can provide enormously secure knowledge or counter-examples when deterministic methods are doomed.

33

34

- All of which is relevant at every level of learning and research. My own works depend heavily on:
 - (i) (High Precision) computation of object(s) for subsequent examination;
 - (ii) Pattern Recognition of Real Numbers (e.g., using CECM's Inverse Calculator* and 'RevEng'), or Sequences (e.g., using Salvy & Zimmermann's 'gfun' or Sloane and Plouffe's Online Encyclopedia); and
 - (iii) Extensive use of Integer Relation $Methods^{\dagger}$: PSLQ & LLL and FFT.

Methods. PSLQ & LLL and FF1.

*ISC space limits have changed from 10Mb being a constraint in 1985 to 10Gb being 'easily available' today.

†Described as one of the top ten "Algorithm's for the Ages," Random Samples, Science, Feb. 4, 2000, [5].

Integer Relation methods are an integral part of a wonderful test bed for experimental mathematics.

• Ruling out things ('exclusion bounds') is, as always in science, often more useful than finding things.



To make more sense of all this it is helpful to discuss the nature of experiment.

Peter Medawar usefully distinguishes four forms of scientific experiment, in his wonderful *Advice to a Young Scientist*, Harper (1979).

FOUR KINDS OF EXPERIMENT

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

The first three forms of experiment are common in mathematics, the fourth (Galilean) is not.

• The Galilean Experiment is also the only one of the four forms which has the promise to make Experimental Mathematics into a serious replicable scientific enterprise.

38

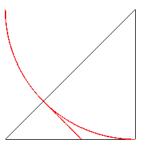
SOME EXAMPLES

Two things about $\sqrt{2}$...

Remarkably one can still find new insights in the oldest areas:

Irrationality. We present graphically, Tom Apostol's lovely new geometric proof* of the irrationality of $\sqrt{2}$.

PROOF. To say $\sqrt{2}$ is rational is to draw a right-angled isoceles triangle with integer sides. Consider the *smallest* right-angled isoceles triangle with integer sides — that is with shortest hypotenuse. Circumscribe a circle of radius the vertical side and construct the tangent on the hypotenuse, as in the picture.



The smaller right-angled isoceles triangle again has integer sides \cdots .

This can be beautifully illustrated in a dynamic geometry package such as *Geometer's Sketch-pad* or *Cinderella*. We can continue to draw smaller and smaller integer-sided similar triangles until the area drops below $\frac{1}{2}$.

• But I give it here to emphasize the ineffably human component of the best proofs, and to suggest the role of the visual.

^{*}*MAA Monthly*, November 2000, 241-242.

• Algebraically: non perfect squares have irrational roots. Indeed if $p/q=\sqrt{n}$ then

$$\frac{p'}{q'} = \frac{n \, q - \left[\sqrt{n}\right] p}{p - \left[\sqrt{n}\right] q} = \frac{p}{q}$$

and 0 < p' < p, 0 < q' < q. (P. Bullen).

ALGORITHMIC vs SYMBOLIC LITERACY?

Newton's method* to compute \sqrt{A} for any (whole) number is the iteration, which makes a 'guess', y at the square root (the solution of $x^2 = A$), and then refines it by replacing y by

$$z = \frac{y + \frac{A}{y}}{2}.$$

Thus, for A = 3, one might guess 2 and get

$$2 \rightarrow \frac{7}{4} \rightarrow \frac{97}{56} \rightarrow \frac{18817}{10864}$$
.

 $(2 \rightarrow 1.75 \rightarrow 1.732142857 \rightarrow 1.7320508075.)$

*One of the most important algorithms in scientific computation can be introduced at exactly this stage.

41

Rationality. $\sqrt{2}$ also makes things rational:

$$(\sqrt{2}^{\sqrt{2}})^{\sqrt{2}} = \sqrt{2}^{(\sqrt{2}\cdot\sqrt{2})} = \sqrt{2}^2 = 2.$$

Hence by the principle of the excluded middle:

either
$$\sqrt{2}^{\sqrt{2}} \in \mathbb{Q}$$
 or $\sqrt{2}^{\sqrt{2}} \not \in \mathbb{Q}$.

In either case we can deduce that there are irrational numbers α and β with α^{β} rational.

But how do we know which ones?

This is not an adequate proof for an Intuitionist or a Constructivist.

• We may build a whole mathematical philosophy project around this.

A classroom experience. This spring I taught this to 100 future elementary school teachers. I spent two full hours on the topic, taught and then gave exactly the prior example on the final with very explicit coaching.

- It is not in the text.
- About 60% attended the lectures.
- About 60% answered correct-ishly.
- Most of the others either did nothing or repeatedly used a 'guess and test' strategy.
 They put in 2, 1.9, 1.8... and compared.
- Thus, those students had no sense of algorithmic or procedural thinking.

42

DISCOVERY vs VERIFICATION

Compare the assertion that

$$\alpha := \sqrt{2} \text{ and } \beta := 2 \ln_2(3) \text{ yield } \alpha^\beta = 3$$
 as Maple confirms.

• This illustrates nicely that verification is often easier than discovery.

Similarly, the fact multiplication is easier than factorization is at the base of secure encryption schemes for e-commerce.

♦ There are eight possible (ir)rational triples:

$$\alpha^{\beta} = \gamma$$
,

and finding examples of all cases is now a fine student project*.

*Note how much can be taught about computation with rational numbers, approximation to irrationals, rates of convergence, etc. from these pieces.

INTEGRALS & PRODUCTS

Even *Maple or Mathematica* 'knows' $\pi \neq \frac{22}{7}$ since

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

though it would be prudent to ask 'why' it can perform the evaluation and 'whether' to trust it?

ullet In this case, computing $\int_0^t \cdots$ provides reassurance.

In contrast, Maple struggles with the following sophomore's dream:

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

• Students asked to confirm this, typically mistake numerical validation for symbolic proof:

$$1.291285997 = 1.291285997$$

45

That said in each case computing adds reality, making concrete the abstract, and making some hard things simple.

• This is strikingly the case in <u>Pascal's Triangle</u>: www.cecm.sfu.ca/interfaces/ which affords an emphatic example where deep fractal structure is exhibited in the elementary binomial coefficients.

David Berlinski* writes

"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." Similarly

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

is rational, while the seemingly simpler (n=2) case

is irrational, indeed transcendental.

• Our Inverse Symbolic Calculator can identify the right-hand side of (2) from it numeric value 0.272029054..., and Maple can 'do' both products.

But the student learns little or nothing from this unless the software can also recreate the steps of a validation. For example, (1) is a lovely telescoping product (or a 'bunch' of Γ -functions.

46

PARTITIONS & PATTERNS

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

(3)
$$1 + \sum_{n>1} p(n)q^n = \frac{1}{\prod_{n\geq 1} (1-q^n)}.$$

Thus, p(5) = 7 since

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

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

Developing (3) is a nice introduction to enumeration via generating functions.

Additive partitions are harder to handle than multiplicative factorizations, but they can be introduced in the elementary school curriculum with questions like:

How many 'trains' of a given length can be built with Cuisenaire rods?

^{*}A sentiment I agree with, unlike others of his, from his "A Tour of the Calculus," Pantheon Books, 1995.

A modern computationally driven question is

How hard is p(n) to compute?

In 1900, the father of combinatorics, Major Percy MacMahon (1854-1929), took months to compute p(200) recursively via (3).

By 2000, Maple would produce p(200) in seconds simply by computing the 200'th term of the series.

• A few years earlier it required one to be careful to compute the series for $\prod_{n\geq 1}(1-q^n)$ first and then to compute the series for the reciprocal of that series!

This seemingly baroque event is occasioned by Euler's pentagonal number theorem

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

49

... from data like

$$P(q) = 1 + q + 2q^{2} + 3q^{3} + 5q^{4} + 7q^{5} + 11q^{6}$$

$$+ 15q^{7} + 22q^{8} + 30q^{9} + 42q^{10} + 56q^{11}$$

$$+ 77q^{12} + 101q^{13} + 135q^{14} + 176q^{15}$$

$$+ 231q^{16} + 297q^{17} + 385q^{18} + 490q^{19}$$

$$+ 627q^{20}b + 792q^{21} + 1002q^{22} + \cdots$$

• If introspection fails, we can find the *pentag-onal numbers* occurring above in *Sloane* and Plouffe's on-line 'Encyclopedia of Integer Sequences':

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

Here we see a very fine example of *Mathematics: the science of patterns* as is the title of Keith Devlin's 1997 book.

• And much more may similarly be done.

The reason is that, if one takes the series for (3) directly, the software has to deal with 200 terms on the bottom.

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

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

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

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

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

and

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

50

CHANGING QUESTIONS

The difficulty of estimating the size of p(n) analytically — so as to avoid enormous computational effort — led to some marvellous mathematical advances by researchers including Hardy and Ramanujan, and Rademacher.

• The corresponding ease of computation may now act as a retardant to mathematical insight. (e.g., Mandated use of "graphing calculators.")

New mathematics is discovered only when prevailing tools run totally out of steam.

⋄ This raises another caveat against mindless computing: will a student or researcher discover structure when it is easy to compute without needing to think about it?

Today, she may thoughtlessly compute p(500) which a generation ago took much, much pain and insight.

Ramanujan typically saw results not proofs and sometimes went badly wrong for that reason.

So will we all.

• Thus, we are brought full face to the challenge — such software should be used, but algorithms must be taught and an appropriate appreciation for and facility with proof developed.

53

• This is, as they say, no coincidence!

While the reasons are too advanced to explain here, it is easy to conduct experiments to discover what happens when $tanh(\pi)$ is replaced by another irrational number, say log(2).

It also affords a great example of fundamental objects that are hard to compute by hand (high precision sums or continued fractions) but easy even on a small computer or calculator.

- \diamond Indeed, I would claim that continued fractions fell out of the undergraduate curriculum precisely because they are too hard to work with by hand.
- And, of course the main message, is again that computation without insight is mind numbing and destroys learning.

HIGH PRECISION FRAUD

Below '[x]' denotes the integer part of x. Consider:

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

is valid to 268 places; while

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

is valid to 12 places. Both are actually transcendental numbers.

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

$$[0,1,\textbf{267},4,14,1,2,1,2,2,1,2,3,8,3,1,\cdots]$$
 and

$$[0, 1, 11, 14, 4, 1, 1, 1, 3, 1, 295, 4, 4, 1, 5, 17, 7, \cdots].$$

54

'PENTIUM FARMING' FOR BITS OF π

Bailey, P. Borwein and Plouffe (1996) discovered a series for π (and corresponding ones for some other *polylogarithmic constants*) which somewhat disconcertingly allows one to compute hexadecimal digits of π without computing prior digits.

The algorithm needs very little memory and no multiple precision. The running time grows only slightly faster than linearly in the order of the digit being computed.

• Until then it was broadly considered impossible to compute digits of such a number without computing most of the preceding ones.

The key, found as described above, 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 by computer using integer relation methods ([3,4,5]) for such a formula.

Once found, it is easy to prove in Mathematica, in Maple or by hand — and provides a very nice calculus exercise. This was a most successful case of

REVERSE MATHEMATICAL ENGINEERING

• This is entirely practicable, God reaches her hand deep into π : in September 1997 Fabrice Bellard (INRIA) used a variant of this formula to compute 152 binary digits of π , starting at the *trillionth position* (10¹²).

Which took 12 days on 20 work-stations working in parallel over the Internet.

57

• In August 1998, Colin Percival (SFU, age 17) similarly made a naturally or "embarrassingly parallel" computation of the *five trillionth bit* (on 25 machines about 10 times the speed of Bellard's). In *hexadecimal notation* he got:

07E45733CC790B5B5979.

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

<u>0</u>0000111110011111.

By September 2000, the *quadrillionth bit* had been found to be '0' (using 250 cpu years on 1734 machines from 56 countries).

• Starting at the 999, 999, 999, 999, 997th bit of π one has:

111000110001000010110101100000110.

58

A CONCRETE SYNOPSIS

I illustrate some of the mathematical challenges with a specific problem, proposed in the *American Mathematical Monthly* (November, 2000), as described in [6].

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

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

- 1. A very rapid Maple computation yielded -0.08406950872765600... as the first 16 digits of the sum.
- 2. The Inverse Symbolic Calculator has a 'smart lookup' feature* that replied that this was probably $-\frac{2}{3} \zeta(\frac{1}{2})/\sqrt{2\pi}$.
- *Alternatively, a sufficiently robust integer relation finder could be used.

- **3.** Ample experimental confirmation was provided by checking this to 50 digits. Thus within minutes we *knew* the answer.
- **4.** As to why? A clue was provided by the surprising speed with which Maple computed the slowly convergent infinite sum.

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

^{*}A search for 'Lambert W function' on MathSciNet provided 9 references — all since 1997 when the function appears named for the first time in Maple and Mathematica.

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

(4)
$$\sum_{k=1}^{\infty} \left(\frac{1}{\sqrt{2\pi k}} - \frac{1}{\sqrt{2}} \frac{(\frac{1}{2})_{k-1}}{(k-1)!} \right) = \frac{\zeta(\frac{1}{2})}{\sqrt{2\pi}},$$

where the binomial coefficients in (4) are those of $\frac{1}{\sqrt{2-2z}}$.

Now (4) is a formula Maple can 'prove'.

6. It remains to show

(5)
$$\sum_{k=1}^{\infty} \left(\frac{k^k}{k! \ e^k} - \frac{1}{\sqrt{2}} \frac{(\frac{1}{2})_{k-1}}{(k-1)!} \right) = -\frac{2}{3}.$$

61

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

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

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

(6)
$$\lim_{z \to 1} \left(\frac{d}{dz} W(-\frac{z}{e}) + \frac{1}{\sqrt{2 - 2z}} \right) = \frac{2}{3}.$$

Again Maple happily does know (6).

8. Of course, this all took a *fair* amount of human mediation and insight.

62

TRUTH vs PROOF

By some accounts Percival's web-computation of π is one of the largest computations ever done. It certainly shows the possibility to use inductive engineering-like methods in mathematics, if one keeps one's eye on the ball.

• To assure accuracy the algorithm can be run twice starting at different points — say starting at 40 trillion minus 10.

The overlapping digits will differ if any error has been made. If 20 hex-digits agree we can argue heuristically that the probability of error is roughly 1 part in 10^{25} .

While this is not a proof of correctness, it is certainly much less likely to be wrong than any really complicated piece of human mathematics.

FERMAT'S MARGINS

For example, perhaps 20 people alive can, given enough time, digest *all* of Andrew Wiles' extraordinarily sophisticated proof of *Fermat's Last Theorem* and it relies on a century long program.

If there is even a 1% chance that each has overlooked the same subtle error* — probably in prior work not explicitly in Wiles' corrected version — then, clearly, many computational based ventures are much more secure.

• This would seem to be a good place to address another common misconception.

No amount of simple-minded case checking constitutes a proof.

^{*}And they may be psychologically predisposed so to do!

FOUR COLOURS SUFFICE

The 1976-7 'proof' of the

Four Colour Theorem. Every planar map can be coloured with four colours so adjoining countries are never the same colour

was a proof because prior mathematical analysis had reduced the problem to showing that a large but finite number of bad configurations could be ruled out.

• The proof was viewed as somewhat flawed because the case analysis was inelegant, complicated and originally incomplete.

In the last few years, the computation has been redone after a more satisfactory analysis.*

*This is beautifully described at www.math.gatech.edu/personal/thomas/FC/fourcolor.html.

65

Though many mathematicians still yearn for a simple proof in both cases, there is no particular reason to think that all elegant true conjectures have accessible proofs.

Nor indeed given Goedel's work need they have proofs at all.

"The message is that mathematics is quasi-empirical, that mathematics is not the same as physics, not an empirical science, but I think it's more akin to an empirical science than mathematicians would like to admit."

(Greg Chaitin, 2000)

66

KUHN & PLANCK

Much of what I have described in detail or in passing involves changing set modes of thinking.

Many profound thinkers view such changes as difficult:

"The issue of paradigm choice can never be unequivocally settled by logic and experiment alone. ... in these matters neither proof nor error is at issue. The transfer of allegiance from paradigm to paradigm is a conversion experience that cannot be forced."

(Thomas Kuhn*)

*In Ed Regis, Who got Einstein's Office? Addison-Wesley, 1986. ... and

"... a new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents die and a new generation grows up that's familiar with it."

(Albert Einstein quoting Max Planck*)

• However hard such paradigm shifts and whatever the outcome of these discourses, mathematics is and will remain a uniquely human undertaking.

*From F.G. Major, The Quantum Beat, Springer, 1998.

HERSH'S HUMANIST PHILOSOPHY

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*.

69

71

- 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 computerassisted 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.

70

- 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.*
- To this I would add that for me now mathematics is not ultimately about proof but about secure mathematical knowledge.

RIEMANN

Georg Friedrich Bernhard Riemann (1826-1866) was one of the most influential thinkers of the past 200 years. Yet he proved very few theorems, and many of the proofs were flawed.

But his conceptual contributions, such as through Riemannian geometry and the Riemann zeta function, and to elliptic and Abelian function theory, were epochal.

^{*}From "Fresh Breezes in the Philosophy of Mathematics," *American Mathematical Monthly*, August-September 1995, 589–594.

IN CONCLUSION

The experimental method is an addition not a substitute for proof, and its careful use is an example of Hersh's 'nontraditional standard of rigor'.

The recognition that 'quasi-intuitive' methods may be used to gain mathematical insight can dramatically assist in the learning and discovery of mathematics.

Aesthetic and intuitive impulses are shot through our subject, and honest mathematicians will acknowledge their role. But a student who never masters proof will not be able to profitably take advantage of these tools.

...FINAL OBSERVATIONS

As we have already seen, the stark contrast between the deductive and the inductive has always been exaggerated. Herbert A. Simon, in his final edition of *The Sciences of the Artificial*, (MIT Press, 1996, page 16) wrote:

"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

13 "... More than fifty years ago Bertrand Russell made the same point about the architecture of mathematics. See the "Preface" to *Principia Mathematica...*

73

74

RUSSELL

"... 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 guite 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."

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

It is precisely this 'post hoc ergo propter hoc' part of theory building that Russell so accurately typifies that makes him an articulate if surprising advocate of my own views.

IN SUMMARY

- Good software packages can make difficult concepts accessible (e.g., Mathematica and Sketchpad) and radically assist mathematical discovery. Nonetheless, introspection is here to stay.
- "We are Pleistocene People" (Kieran Egan). Our minds can subitize, but were not made for modern mathematics. We need all the help we can get.
- While proofs are often out of reach to students or indeed lie beyond present mathematics, understanding, even certainty, is not.
- "it is more important to have beauty in one's equations than to have them fit experiment." (Paul Dirac)
- And surely: 'You can't go home again.' (Thomas Wolfe)

Old questions are solved by disappearing, evaporating, while new questions corresponding to the changed attitude of endeavor and preference take their place. Doubtless the greatest dissolvent in contemporary thought of old questions, the greatest precipitant of new methods, new intentions, new problems, is the one effected by the scientific revolution that found its climax in

• Quoted from *The Influence of Darwin on Philosophy*, 1910.

the "Origin of Species." "

JOHN DEWEY

" Old ideas give way slowly; for they are more than abstract logical forms and categories. They are habits, predispositions, deeply engrained attitudes of aversion and preference. Moreover, the conviction persists-though history shows it to be a hallucination that all the questions that the human mind has asked are questions that can be answered in terms of the alternatives that the questions themselves present. But in fact intellectual progress usually occurs through sheer abandonment of questions together with both of the alternatives they assume an abandonment that results from their decreasing vitality and a change of urgent interest. We do not solve them: we get over them.

78

APPENDIX: INTEGER RELATIONS

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

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

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

- (n = 2) Euclid's algorithm gives solution.
- $(n \ge 3)$ Euler, Jacobi, Poincaré, 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.

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.

81

FINALIZING FORMULAE

♦ If we know or suspect an identity exists integer relations are very powerful.

 (Machin's Formula) We try lin_dep on [arctan(1), arctan(1/5), arctan(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 Formula). We try lin_dep on $[\arctan(1),\arctan(1/2),\arctan(1/5),\arctan(1/8)]$ 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 to compute 200 digits of π

82

ZETA FUNCTIONS

• The zeta function is defined, for s > 1, by

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

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

$$S_2 := \zeta(2) = 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k}}$$

$$A_3 := \zeta(3) = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^3 \binom{2k}{k}}$$

$$S_4 := \zeta(4) = \frac{36}{17} \sum_{k=1}^{\infty} \frac{1}{k^4 \binom{2k}{k}}$$

♦ These results 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

in his head.)

ullet 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:

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

$$- \frac{4}{3}L^5 + \frac{8}{3}L^3\zeta(2) + 4L^2\zeta(3)$$

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

where $L:=\log(\rho)$ and $\rho:=(\sqrt{5}-1)/2$; with similar formulae for A_4,A_6,S_5,S_6 and $S_7.$

- A less known formula for $\zeta(5)$ due to Koecher suggested generalizations for $\zeta(7), \zeta(9), \zeta(11) \ldots$
- ♦ 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:

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

• 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,

$$\sum_{n=1}^{\infty} \zeta(4n+3)z^{4n}$$
(8)
$$= \sum_{k=1}^{\infty} \frac{1}{k^3(1-z^4/k^4)}$$

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

- ♦ 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 (7).

85

HOW IT WAS FOUND

♦ The first ten cases show (8) has the form

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

for undetermined P_k ; with abundant data to compute

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

• We found many reformulations of (8), including a marvelous finite sum:

(9)
$$\sum_{k=1}^{n} \frac{2n^2}{k^2} \frac{\prod_{i=1}^{n-1} (4k^4 + i^4)}{\prod_{i=1, i \neq k}^{n} (k^4 - i^4)} = {2n \choose n}.$$

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

- \bullet This identity was recently proved by Almkvist and Granville (Experimental Math, 1999) thus finishing the proof of (8) and giving a rapidly converging series for any $\zeta(4N+3)$ where N is positive integer.
- \diamond And perhaps shedding light on the irrationality of $\zeta(7)$? Recall that $\zeta(2N+1)$ is not proven irrational for N>1: though one of $\zeta(2n+3)$ for n=1,2,3,4 is.
- † Paul Erdos, when shown (9) shortly before his death, rushed off. Twenty minutes later he returned saying he did not know how to prove it but if proven it would have implications for Apéry's result (' ζ (3) is irrational').