Integer Relation Methods : An Introduction

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CARMA

THE UNIVERSITY OF NEWCASTLE AUSTRALIA

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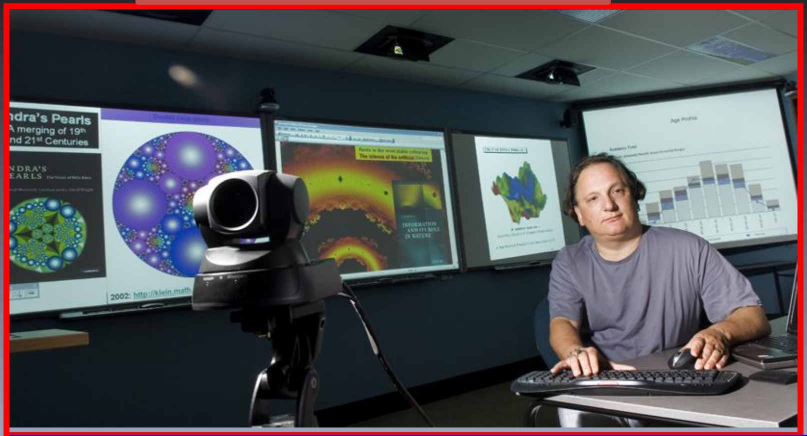
ABSTRACT



Jonathan M. Borwein

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Computer Assisted Research Mathematics and its Applications (CARMA)

Integer Relation Methods were named as one of the 'top ten' algorithms of the 20th century by Computers in Science and in Engineering (1999).

In my talk I will outline what Integer Relation Methods are and I will illustrate their remarkable utility on a variety of mathematical problems, some pure and some applied.

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

ΣOPT

Australian and New Zealand
Industrial and Applied Mathematics

Optimization Group

Optimization Group is a special interest group of ANZIAM. The group consists of a forum for Australian and New Zealand optimization specialists to interact. The Optimization group holds annual meetings: the Optimization Annual Workshop.

The Optimization group brings together scientists from Australia and New Zealand in order to:

- Maintain, promote and further develop the theory and practice of optimization and optimal control;
- Attract students to the discipline.

Rules of Procedure

Optimization - Optimization Group Rules

Optimization Group Executive

Chair: Jonathan Borwein (University of Newcastle) Secretary: Regina Burachik (University of South Australia) Treasurer: Andrew Eberhard (Royal Melbourne Institute of Technology)

Committee: to be elected

Conferences

The first Annual Conference of Optimization will be held at the Centre for Computer Assisted Mathematical Research and Applications at the University of Newcastle in February.

Fully refereed proceedings will be produced from each conference and will be available for purchase

Relevant Conferences

Relevant Books

Relevant Sites

Optimization Group
Optimization Group Rules

INTEGER RELATION ALGORITHMS: WHAT THEY ARE

Let (x_n) be a vector of real numbers. An **integer relation algorithm** finds integers (a_n) such that

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

or provides an **exclusion bound**

- i.e., testing linear independence over **Q**

- At present, the PSLQ algorithm of mathematician-sculptor *Helaman Ferguson* is the **best** known integer relation algorithm.
- High precision arithmetic software is required: at least $d \times n$ digits, where d is the size (in digits) of the largest of the integers a_k.

INTEGER RELATION ALGORITHMS: HOW THEY WORK

Let (x_n) be a vector of real numbers. An **integer relation algorithm** finds integers (a_n) such that

$$a_1x_1 + a_2x_2 + \cdots + a_nx_n = 0$$

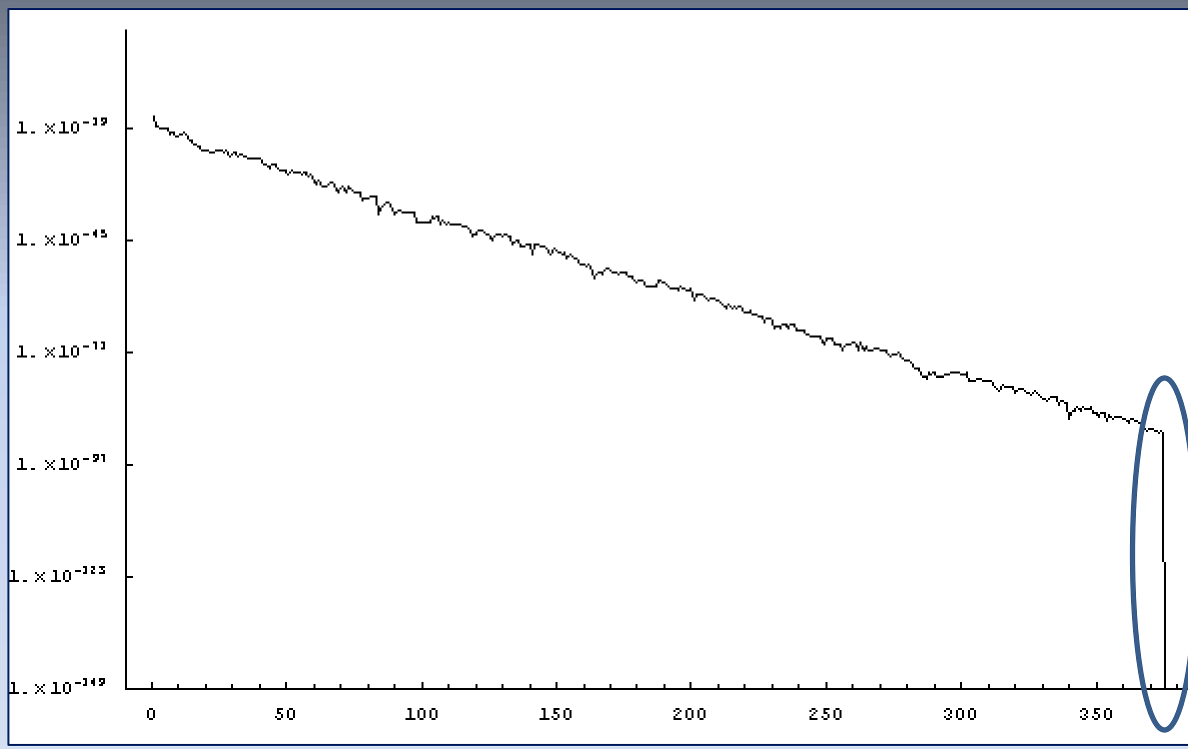
or provides an **exclusion bound.**

PSLQ operates by developing, iteratively, an integer matrix A that successively reduces the maximum absolute value of the entries of the vector $y = Ax$, until one of the entries of y is either zero or within roughly 10^{-p} of zero, where p is the numeric precision used.

Any integer relation detection scheme needs data to at least nd-digit precision: via a simple pigeonhole analysis. Assume the x vector does not satisfy an integer relation, with $|x_j| \leq 1$. Suppose all a_j satisfy $|a_j| \leq 10^d$. Then $\sum_{1 \leq j \leq n} a_j x_j$ will assume one of $2^n 10^{nd}$ values in $[-n10^d, n10^d]$, depending on a. The average distance between these values is $2n2^{-n}10^{d-nd}$. Thus, an interval of size 10^{-p} around zero is likely to contain a spurious "relation" unless p is significantly larger than $nd - d$.

INTEGER RELATION ALGORITHMS: HOW THEY WORK

PSLQ is a combinatorial optimization algorithm designed for (pure) mathematics



The method is “self-diagnosing”---- the error drops precipitously when an identity is found. And basis coefficients are “small”.

TOP TEN ALGORITHMS

▶ 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.

- integer relation detection (PSLQ, 1997) was the most recent of the top ten

HELAMAN FERGUSON
SCULPTOR and MATHEMATICIAN

PROFILE: HELAMAN FERGUSON

Carving His Own Unique Niche, In Symbols and Stone

By refusing to choose between mathematics and art, a self-described "misfit" has found the place where parallel careers meet

BALTIMORE, MARYLAND—Helaman Ferguson's sculpture studio is set back from the road, hidden behind a construction site. Inside, pieces of art line shelves and cover tabletops. Ferguson, clad in a yellow plastic apron and a black T-shirt, serenely makes his way through the room. The 66-year-old is tall and white-haired, his bare arms revealing a strength requisite for his avocation.

The most striking work in the studio is a more than 2-meter-tall, 5-ton chunk of granite. When it is finished, it will stand in the entry to the science building at Macalester College in St. Paul, Minnesota. Right now, it is a mass of curving surfaces sloping in different directions, its surface still jagged with the rough grains left by the diamond-toothed chainsaw Ferguson uses to carve through the stone.

"I'm in my negative-Gaussian-curvature phase," Ferguson says. "Say we're going to shake hands, but we don't quite touch. OK, see the space between the two hands?" That saddle-shaped void, he explains, is a perfect example of negative Gaussian curvature. Our bodies contain many others, he adds: the line between the first finger's knuckle and the wrist, for instance, and where the neck meets the shoulders.

The topological jargon is no surprise: Ferguson spent 17 years as a mathematics professor at Brigham Young University (BYU) in Provo, Utah. What is unusual is how successfully he has pursued a dual career as mathematician and artist and the ease with which he blurs the categories. Math inspires and figures in almost all of Ferguson's artistic works. Through them, he has helped some mathematicians appreciate the artist's craft and aesthetic. And he's persuaded perhaps even more artists that math may not be as frighteningly elusive as they believe, or even if it is out of their reach, it's as beautiful as any work of art they might imagine. "The way he has brought together the worlds of science and the arts—this is an admirable thing," says Harvey Bricker, Ferguson's former college roommate.

Function-al form. The Fibonacci Fountain at the Maryland Science and Technology Center was inspired by the "golden ratio."

Twin callings

Ferguson himself finds it hard to say which calling came first. As a teenager in upstate New York, he learned stone carving as an informal apprentice to his adopted father, a stonemason. Artistically, however, he was more drawn to painting. After finishing high school in 1958, he wanted to study art as well as math. He chose Hamilton College, a liberal arts school in upstate New York near where he had spent most of his childhood, where he could do both.

After getting his math degree, he enrolled in a doctoral program in math at the University of Wisconsin, Madison. He paid for some of his living expenses by selling paintings. He also met and began dating an undergraduate art student, Claire. The couple married in 1963 and had their first child (of an eventual seven) in 1964. Ferguson dropped out of school for a couple of years to work as a computer programmer, then resumed his math studies. He obtained his master's degree in mathematics at BYU and a doctorate in group representations—a broad area of math that involves algebra, geometry, topology, and analysis—at the University of Washington, Seattle. In 1971, he accepted an appointment as assistant professor at BYU.

As a mathematician, Ferguson is perhaps best known for the algorithm he developed with BYU colleague Rodney Forcade. The algorithm, called PSLQ, finds mathematical relations among seemingly unrelated real numbers. Among many other applications, PSLQ provided an efficient way of computing isolated digits within pi and blazed a path for modeling hard-to-calculate particle interactions in quantum physics.

In 2000, the journal *Computing in Science and Engineering* named it one of the top 10 algorithms of the 20th century.

Meanwhile, Ferguson's artistic career also developed apace. When he married Claire, a painter, the two struck a deal: "I get the floors, she gets the walls," he says. He began focusing more on sculpture. The art department at BYU allotted him some studio space, and he turned out a regular stream of work. He's done commissions for the Maryland Science and Technology Center, the University of California, Berkeley, the University of St. Thomas in St. Paul, and many other institutions. He has also designed small sculptures for awards presented by the Clay Mathematics Institute in Cambridge, Massachusetts, the Canadian Mathematical Society in Ontario, and the Association for Computing Machinery in New York City.

CREDITS: J. MIOGLIA/SCIENCE

Published by AAAS

He has worked to keep a foot in each of the "two cultures." While at BYU, he taught a course each year for honors students called Qualitative Mathematics and Its Aesthetics. Both art students and math students enrolled: the artists looking for a palatable way to take in a math requirement, and the math students lured by the promise of higher level mathematics. Ferguson delivered on both ends. He taught concepts mathematicians don't normally encounter until graduate school, such as braid theory. Artists could relate to braids as physical objects, rope or hair that can be woven into a specific form. But students were also asked to write down an algebra to go along with how the braid was formed—a noncommutative algebra.

"Some of these folks were in there because they were either afraid of or hated math," says Ferguson. At the end of the semester, however, "quite a few art students wanted a follow-on semester—more math, more art."

Bridging

Ferguson, who left BYU in 1988, now devotes most of his time to his art. For his large-scale or complicated pieces, he uses computer programs such as Mathematica to form and refine the shape he wants the finished piece to take. "With sculpture, you want a piece to be a unit so it has direct impact as a form," he says. "Sculptures are complicated enough already." With computer programs, he says, before even putting hand to stone "you can walk around [the piece] and see a different view; you can touch it and reshape it to make it simpler and more direct."

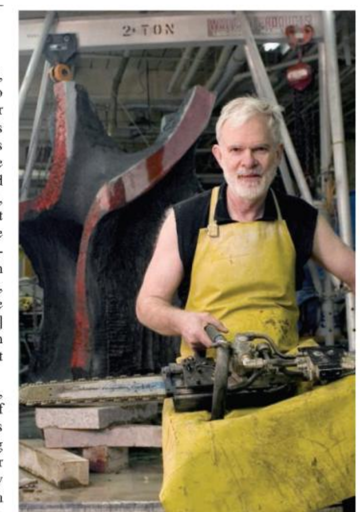
Once the design is in place, Ferguson turns to the task of carving the stone. He works alone, without assistants, using both chisels and assorted power tools. Finally comes a lengthy smoothing process, going from 20-grit sandpaper to as fine as 8500-grit. Ferguson has to work "wet" much of the time, using water to wash down the fine particles of stone that could otherwise become deposited in his lungs. For some of the work, he dons gloves made of woven stainless steel and a positive-pressure facemask. A large sculpture can take several months to complete, working flat-out.

Twisted. Braids and knots turn up in many of Ferguson's works, including these small metal sculptures

Granite is Ferguson's favorite medium. "Mathematics is kind of timeless," he says, "so incorporating mathematical themes and ideas into geologically old stone—that's something that has great aesthetic appeal to me." He also likes the idea that his sculptures will be around for millions or even billions of years.

The finished sculptures vary widely in appearance. Some are delicate, with looped projections or intricate imprints, and are small enough to hold in one's hand. Others are massive, meant to be touched, even climbed on (as many children have discovered). As a rule, they also contain much more detail than meets the eye. "My work generally involves a circle of ideas," says Ferguson. People he interacts with, new information he obtains, mathematics he has had on his mind—all of these become "part of the design consideration."

As an example, he cites an architectural-scale sculpture recently installed outside his alma mater Hamilton College's new science building. The work, made of 10-centimeter-thick granite, centers on a pair of massive disks representing the planets Mars and Venus. "Venus" is exactly 161 centimeters in diameter—the height of the average female Hamilton student, taken from the records of one of the college's psychology professors. "Mars" is 174 centimeters in diameter—the average male student's height. The disks are inlaid with tiles in a pattern defined by the Poincaré and Beltrami-Klein models of plane hyperbolic geometry.



Tough medium. A diamond-toothed chainsaw helps Ferguson carve through granite rocks that are up to a billion years old.

CREDITS: J. MIOGLIA/SCIENCE

Ferguson's admirers say his artwork goes far beyond academic exercises. David Broadhurst, a physicist at the Open University in Milton Keynes, U.K., learned about Ferguson's sculpture after using the PSLQ algorithm in his research in quantum mechanics. He compares Ferguson's artistic renderings of math to Fournier playing the Bach cello suites, "giving expression to abstract forms, whose beauty is preexistent to the interpretation, yet recreated in a widely accessible medium."

For his part, Ferguson says his lifelong project to embody mathematics in mass and form is very much in the spirit of the times—and he credits technology with making it all possible. "We're living in the golden age of art, we really are. But it's also the golden age of science," he says. "Today, young people have seen more art and science in, say, their first 25 years of life than anyone in the years before that." With the collaborations between computer scientists and artists, and tools for art being used as tools for scientific exploration and invention, Ferguson suggests we may be in the midst of a second Renaissance. "It's a great time to be alive," says Ferguson, "because there are more places for misfits like myself to survive."

–KATHERINE UNGER

Katherine Unger is a writer in Washington, D.C.

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Peter Borwein
in front of
Helaman Ferguson's
work

CMS Meeting
December 2003
SFU Harbour Centre

Ferguson uses high tech tools and micro engineering at NIST to build monumental math sculptures

MADELUNG's CONSTANT

David Borwein CMS Career Award

$$= \sum_{n,m,p}{}' \frac{(-1)^{n+m+p}}{\sqrt{n^2+m^2+p^2}}$$

This polished solid silicon bronze sculpture is inspired by the work of David Borwein, his sons and colleagues, on the conditional series above for salt, Madelung's constant. This series can be summed to uncountably many constants; one is Madelung's constant for **electro-chemical stability of sodium chloride**.

This constant is a period of an elliptic curve, a real surface in four dimensions. There are uncountably many ways to imagine that surface in three dimensions; one has negative gaussian curvature and is the tangible form of this sculpture. (As described by the artist.)


THEORIES
PROOFS
S. Harris

INTEGER RELATION ALGORITHMS: WHAT THEY DO: ELEMENTARY EXAMPLES

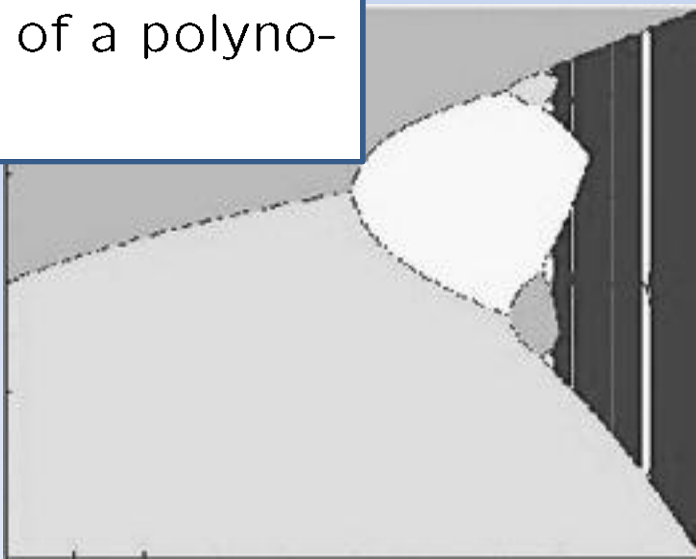
ALGEBRAIC NUMBERS

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.

An application was to determine explicitly the 4th and 5th bifurcation points of the logistics curve have degrees 256.



FINALIZING FORMULAE

- If we suspect an identity PSLQ is powerful.

- (*Machin's Formula*) We try PSLQ 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).]

If we try with arctan(1/238) we obtain huge integers

- (*Dase's 'mental' Formula*) We try PSLQ 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.]

In his head

INTEGER RELATIONS in MAPLE

```
> with(IntegerRelations);Digits:=25;
```

$$[LLL, LinearDependency, PSLQ]$$

$$Digits := 25 \qquad (2)$$

```
> PSLQ([Pi,arctan(1/2),arctan(1/5),arctan(1/8)]);
```

$$[1, -4, -4, -4] \qquad (3)$$

```
> PSLQ([Pi,arctan(1/2),arctan(1/5),arctan(1/9)]);
```

$$[10129, 2473744, -4734091, -2207521] \qquad (4)$$

```
> pslq(Pi,[arctan(1/2),arctan(1/5),arctan(1/8)]);
```

$$[1, 4, 4, 4], \text{"Error is"}, -2.\ 10^{-35}, \text{"checking to"}, 35, places$$

$$\pi = 4\arctan\left(\frac{1}{2}\right) + 4\arctan\left(\frac{1}{5}\right) + 4\arctan\left(\frac{1}{8}\right) \qquad (5)$$

```
> a:=evalf(sqrt(3)+sqrt(5));identify(a);
```

$$a := 3.968118785068666989936620$$

$$\sqrt{3} + \sqrt{5} \qquad (6)$$

```
> ?identify
```

- *Maple* also implements the Wilf-Zeilberger algorithm
- *Mathematica* can only recognize algebraic numbers

INTEGER RELATION ALGORITHMS: WHAT THEY DO: ADVANCED EXAMPLES

- THE BBP FORMULA FOR PI
- PHYSICAL INTEGRALS
  - ISING AND QUANTUM FIELD THEORY
- APERY SUMS
  - AND GENERATING FUNCTIONS
- RAMANUJAN SERIES FOR $1/\pi^N$

The BBP FORMULA for Pi

In 1996 Bailey, P. Borwein and Plouffe, using PSLQ for months, discovered this formula for π:

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

Indeed, this formula permits one to directly calculate binary or hexadecimal (base-16) digits of π beginning at an arbitrary starting position n, without needing to calculate any of the first n-1 digits.

A finalist for the **Edge of Computation Prize**, it has been used in compilers, in a record web computation, and in a trillion-digit computation of Pi.

PHYSICAL INTEGRALS (2006-2008)

The following integrals arise independently in mathematical physics in Quantum Field Theory and in Ising Theory:

$$C_n = \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

We first showed that this can be transformed to a 1-D integral:

$$C_n = \frac{2^n}{n!}\int_0^\infty t K_0^n(t)\ dt$$

where K_0 is a **modified Bessel function**. We then (with care) computed 400-digit numerical values (over-kill but who knew), from which we found with **PSLQ** these (now proven) **arithmetic** results:

$$C_3 = L_{-3}(2) := \sum_{n\geq 0} \left\{ \frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right\}$$

$$C_4 = \frac{7}{12}\zeta(3)$$

$$\lim_{n\to\infty} C_n = 2e^{-2\gamma}$$

IDENTIFYING THE LIMIT WITH THE **ISC** (2.0)

We discovered the limit result as follows: We first calculated:

$$C_{1024} \; = \; 0.63047350337438679612204019271087890435458\ldots$$

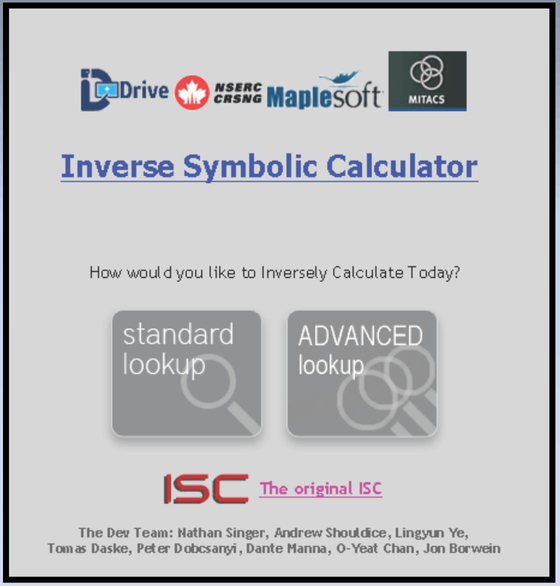
We then used the Inverse Symbolic Calculator, the online numerical constant recognition facility available at:
http://ddrive.cs.dal.ca/~isc/portal

Output: **Mixed constants, 2 with elementary transforms.**

.6304735033743867 = sr(2)^2/exp(gamma)^2

In other words,

$$C_{1024} \; \approx \; 2e^{-2\gamma}$$



References. Bailey, Borwein and Crandall, “Integrals of the Ising Class," *J. Phys. A.*, **39** (2006)
Bailey, Borwein, Broadhurst and Glasser, “Elliptic integral representation of Bessel moments," *J. Phys. A,* **41** (2008) [IoP Select]

APERY-LIKE SUMMATIONS

The following formulas for ζ(s) have been known for many decades:

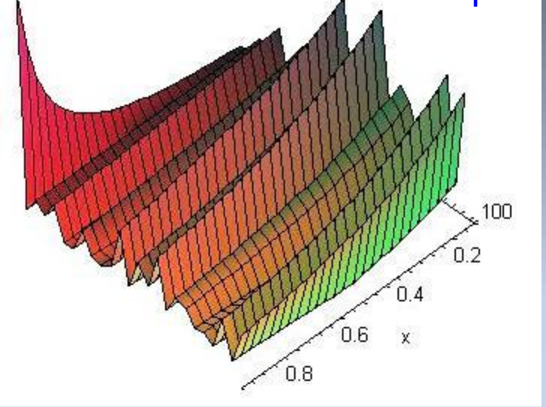
$$\zeta(2) = 3\sum_{k=1}^{\infty}\frac{1}{k^2\binom{2k}{k}},$$

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

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

for $\mathrm{Re}(s) > 1$
$\zeta(s) := \sum_{n=1}^{\infty}\frac{1}{n^s}$

The RH in Maple



These results have led many to speculate that

$$Q_5 := \zeta(5)/\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}}$$

might be some nice rational or algebraic value.

Sadly (?), PSLQ calculations have established that if Q_5 satisfies a polynomial with **degree** at most **25**, then at least **one coefficient** has **380** digits. But positive results exist.

APERY OGF'S

1. via PSLQ to 5,000 digits (120 terms)

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

$$\zeta(2) = \frac{\pi^2}{6}, \zeta(4) = \frac{\pi^4}{90}, \zeta(6) = \frac{\pi^6}{945}, \ldots$$

Euler (1707-73)

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

$$= \sum_{k=0}^{\infty} \zeta(2k+2)x^{2k} = \sum_{n=1}^{\infty} \frac{1}{n^2-x^2}$$

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

1

2. reduced as hoped

2

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

2005 Bailey, Bradley & JMB *discovered and proved* - in 3Ms - three *equivalent* binomial identities

3

$${}_3F_2\left(\begin{matrix}3n, n+1, -n \\ 2n+1, n+1/2\end{matrix}; \frac{1}{4}\right) = \frac{\binom{2n}{n}}{\binom{3n}{n}}$$

3. was easily computer proven (Wilf-Zeilberger) **(now 2 human proofs)**

NEW RAMANUJAN-LIKE IDENTITIES

Guillera (around 2003) found Ramanujan-like identities, including:

$$\frac{128}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (13 + 180n + 820n^2) \left(\frac{1}{32}\right)^{2n}$$

$$\frac{8}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (1 + 8n + 20n^2) \left(\frac{1}{2}\right)^{2n}$$

$$\frac{32}{\pi^3} \stackrel{?}{=} \sum_{n=0}^{\infty} r(n)^7 (1 + 14n + 76n^2 + 168n^3) \left(\frac{1}{8}\right)^{2n}.$$

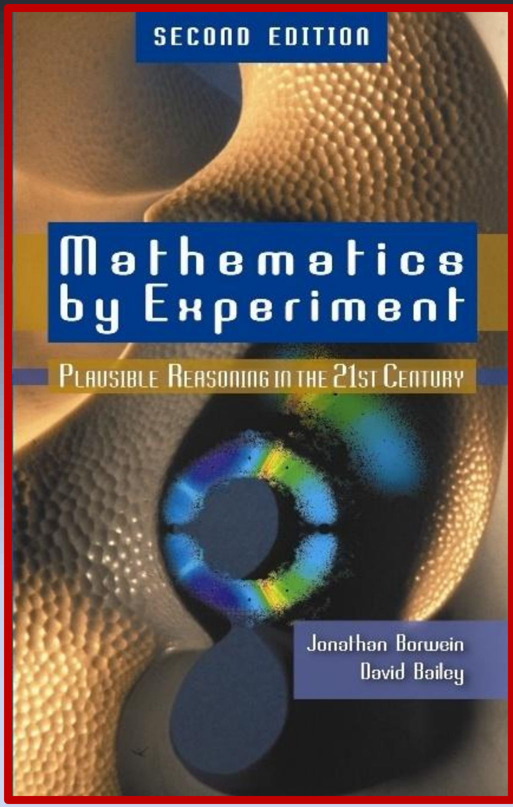
where

$$r(n) = \frac{(1/2)_n}{n!} = \frac{1/2 \cdot 3/2 \cdot \cdots \cdot (2n-1)/2}{n!} = \frac{\Gamma(n+1/2)}{\sqrt{\pi}\,\Gamma(n+1)}$$

Guillera proved the first two using the Wilf-Zeilberger algorithm. He ascribed the third to Gourevich, who found it using integer relation methods. **It is true but has no hint of a proof…**

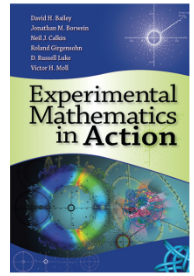
As far as we can tell there are no higher-order analogues!

REFERENCES



Experiencing Experimental Mathematics

Experimental Mathematics in Action
David H. Bailey, Jonathan M. Borwein, Neil J. Calkin, Roland Girgensohn, D. Russell Luke, Victor H. Moll



"David H. Bailey et al. have done a fantastic job to provide very comprehensive and fruitful examples and demonstrations on how experimental mathematics acts in a very broad area of both pure and applied mathematical research, in both academic and industry. Anyone who is interested in experimental mathematics should, without any doubt, read this book!"
—*Gazette* of the Australian Mathematical Society

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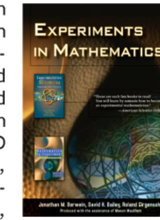
Jonathan M. Borwein, David H. Bailey, Roland Girgensohn

In the short time since the first edition of *Mathematics by Experiment: Plausible Reasoning in the 21st Century* and *Experimentation in Mathematics: Computational Paths to Discovery*, there has been a noticeable upsurge in interest in using computers to do real mathematics. The authors have updated and enhanced the book files and are now making them available in PDF format on a CD-ROM. This CD provides several "smart" features, including hyperlinks for all numbered equations, all Internet URLs, bibliographic references, and an augmented search facility assists one with locating a particular mathematical formula or expression.



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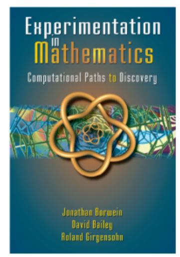
Computational Paths to Discovery
Jonathan M. Borwein, David H. Bailey, Roland Girgensohn



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Plausible Reasoning in the 21st Century
Jonathan M. Borwein, David H. Bailey

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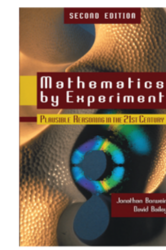

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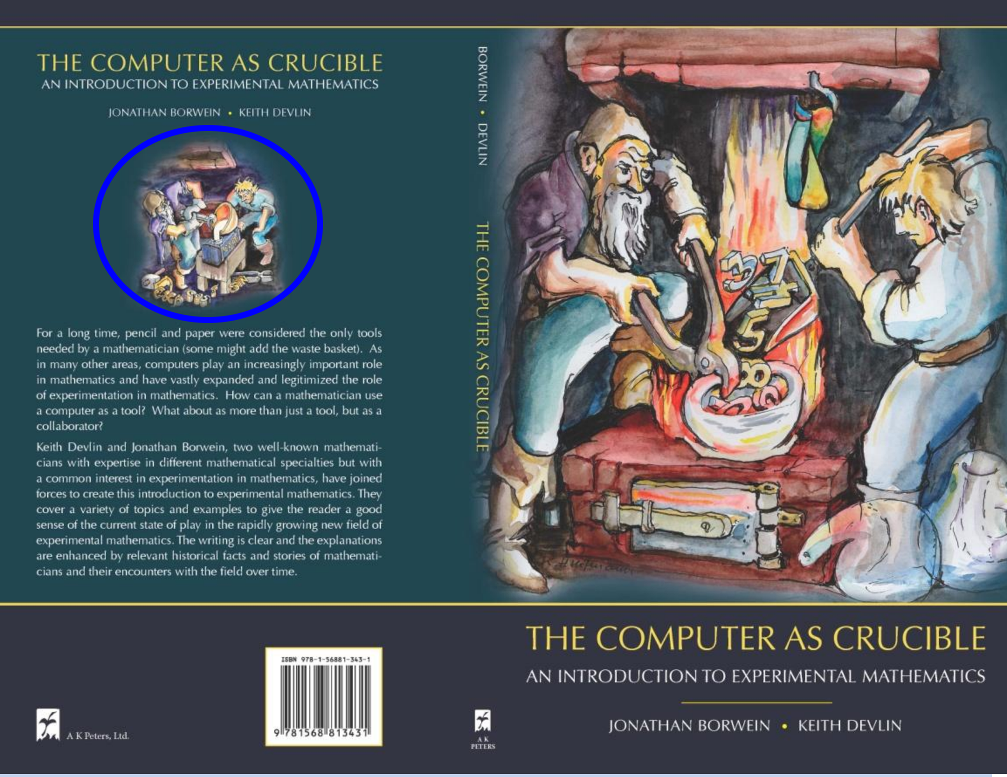

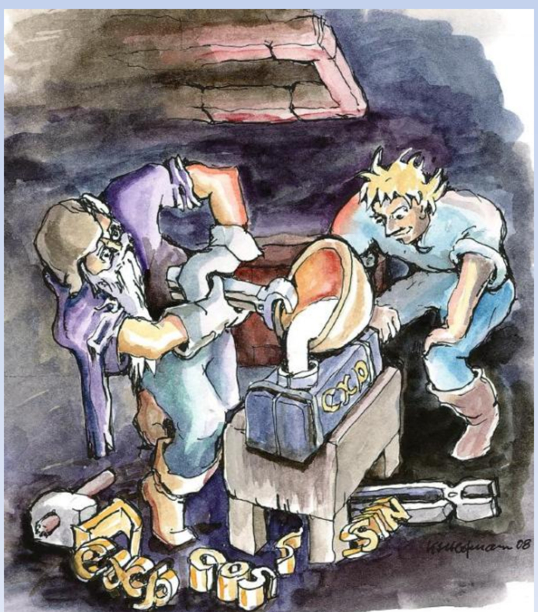

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