

Digitally-assisted Discovery and Proof

Two Lectures on Experimental Mathematics
(ANU, November 13-14, 2008)



Jonathan Borwein, FRSC

www.cs.dal.ca/~jborwein



Canada Research Chair in Collaborative Technology
Laureate Professor Newcastle, NSW

“intuition comes to us much earlier and with much less outside influence than formal arguments which we cannot really understand unless we have reached a relatively high level of logical experience and sophistication.

Therefore, I think that in teaching high school age youngsters we should emphasize intuitive insight more than, and long before, deductive reasoning.”

George Polya (1887-1985)



THE UNIVERSITY OF
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Revised 16/10/08

ABSTRACT

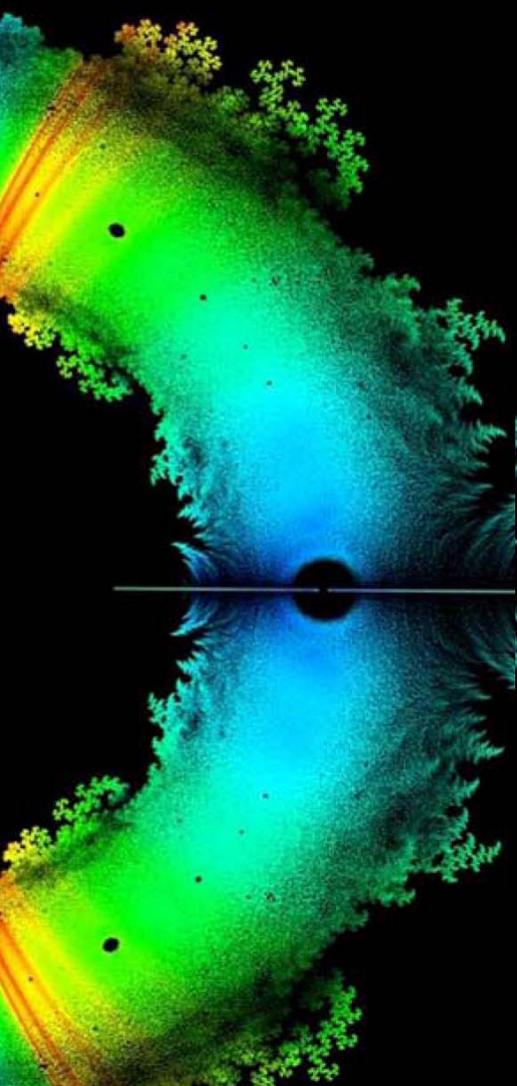


Jonathan M. Borwein
Dalhousie and Newcastle

I will argue that the mathematical community (appropriately defined) is facing a great challenge to re-evaluate the role of proof in light of the power of current computer systems, of modern mathematical computing packages and of the growing capacity to data-mine on the internet. With great challenges come great opportunities. I intend to illustrate the current challenges and opportunities for the learning and doing of mathematics.

“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 (1865-1963)

COMPUTER ASSISTED RESEARCH MATHEMATICS AND ITS APPLICATIONS (CARMA)



OVERVIEW

Two decades ago, few mathematicians used computations in serious research work. There was a wide-spread view that “real mathematicians don’t compute.” In the ensuing years, computer hardware has skyrocketed in power and plunged in cost, thanks to the remarkable persistent phenomenon of Moore’s Law. And many powerful mathematical software products have emerged. Just as importantly, a new generation of mathematicians is eager to use these tools. Thus, many new results are being discovered, and use of mathematics in society is expanding rapidly.

Experimental methodology provides a compelling way to build insight, to find and confirm or confront conjectures; to make mathematics more tangible, lively and fun for a researcher, a practitioner, or a novice. Experimental approaches also broaden the interdisciplinary nature of research: a chemist, physicist, engineer, and mathematician may not understand each others’ motivation or jargon, but often share underlying computational tools, usually to the benefit of all parties.

Advanced mathematical computation is equally essential to solution of real-world problems; sophisticated mathematics is core to software used by decision-makers, engineers, scientists, managers, and who design, plan and control the products and systems key to present day life.

NEWCASTLE RESEARCH CENTRE (7 core members)

OBJECTIVES

- To perform research and development relating to the informed use of computers as an adjunct to mathematical discovery (including current advances in cognitive science, in information technology, operations research and theoretical computer science).
- To perform research and development of mathematics underlying computer-based decision support systems, particularly in automation and optimization of scheduling, planning and design activities, and to undertake mathematical modelling of such activities.
- To promote and advise on the use of appropriate tools (hardware, software, databases, learning object repositories, mathematical knowledge management, collaborative technology) in academia, education and industry.
- To make University of Newcastle a world-leading institution for Computer Assisted Research Mathematics and its Applications.

OUTLINE

- ◆ Working Definitions of:
 - Discovery
 - Proof (and Maths)
 - Digital-Assistance
 - Experimentation (in Maths and in Science)

- ◆ Five Core Examples:
 - What is that number?
 - Why Pi is not $22/7$
 - Making abstract algebra concrete
 - A more advanced foray into mathematical physics
 - A dynamical system I can visualize but not prove

- ◆ Making Some Tacit Conclusions Explicit

- ◆ Three Additional Examples (as time permits)
 - Integer Relation Algorithms
 - Wilf-Zeilberger Summation
 - A Cautionary Finale

WHAT is a DISCOVERY?

“discovering a truth has three components. First, there is the independence requirement, which is just that one comes to believe the proposition concerned by one’s own lights, without reading it or being told. Secondly, there is the requirement that one comes to believe it in a reliable way. Finally, there is the requirement that one’s coming to believe it involves no violation of one’s epistemic state. ...

In short, discovering a truth is coming to believe it in an independent, reliable, and rational way.

Marcus Giaquinto, *Visual Thinking in Mathematics. An Epistemological Study*, p. 50, OUP 2007

- **Leading to** “secure mathematical knowledge”?

“All truths are easy to understand once they are discovered; the point is to discover them.” – Galileo Galilei

WHAT is a PROOF?

“PROOF, *n.* a sequence of statements, each of which is either validly derived from those preceding it or is an axiom or assumption, and the final member of which, the *conclusion*, is the statement of which the truth is thereby established. A *direct proof* proceeds linearly from premises to conclusion; an *indirect proof* (also called *reductio ad absurdum*) assumes the falsehood of the desired conclusion and shows that to be impossible. See also **induction, deduction, valid.** ”

Collins Dictionary of Mathematics

“No. I have been teaching it all my life, and I do not want to have my ideas upset.”
- Isaac Todhunter (1820 - 1884) recording **Maxwell's response** when asked whether he would like to see an experimental demonstration of conical refraction.

Not to Mention Formal Proof

Often quite far in ambit from my own preoccupations

Coming of age as December **Notices of the AMS** make clear:

“We can assert with utmost confidence that the error rates of top-tier theorem-proving systems are orders of magnitude lower than error rates in the most prestigious mathematical journals. Indeed, since a formal proof starts with a traditional proof, then does strictly more checking even at the human level, it would be hard for the outcome to be otherwise.”
[Hales, p. 1376]

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Features

A Special Issue on Formal Proof

Using computers in proofs both extends mathematics with new results and creates new mathematical questions about the nature and technique of such proofs. This special issue features a collection of articles by practitioners and theorists of such formal proofs which explore both aspects.

Formal Proof
Thomas Hales
(pp. 1370)
[✉ Email this](#)

Formal Proof--The Four-Color Theorem
Georges Gonthier
(pp. 1382)
[✉ Email this](#)

Formal Proof--Theory and Practice
John Harrison
(pp. 1395)
[✉ Email this](#)

Formal Proof--Getting Started
Freek Wiedijk

Communications

WHAT IS...a Period Domain?
James Carlson and Phillip Griffiths

Adventures in Academic Year Undergraduate Research
Kathryn Leonard

Commentary

Letter from the Editor
Job Talk
Andy Magid

Letters to the Editor
Mathematical Omnibus and Roots to Research
A Book Review
Reviewed by Harriett Pollatsek

The Wraparound Universe
A Book Review
Reviewed by George F. R. Ellis

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MacKichan Software,

WHAT is MATHEMATICS?

mathematics, n. a group of related subjects, including algebra, geometry, trigonometry and calculus, concerned with the study of number, quantity, shape, and space, and their inter-relationships, applications, generalizations and abstractions.

- ◆ This definition--from my *Collins* Dictionary has no mention of proof, nor the means of reasoning to be allowed (vidé Giaquinto). *Webster's* contrasts:

induction, n. any form of reasoning in which the conclusion, though supported by the premises, does not follow from them necessarily.

and

deduction, n. **a.** a process of reasoning in which a conclusion follows necessarily from the premises presented, so that the conclusion cannot be false if the premises are true.

b. a conclusion reached by this process.

“If mathematics describes an objective world just like physics, there is no reason why inductive methods should not be applied in mathematics just the same as in physics.”

- Kurt Gödel (1951 Gibbs Lecture)

-echoes of Quine

WHAT is DIGITAL ASSISTANCE?

- ◆ Use of Modern Mathematical Computer Packages
 - Symbolic, Numeric, Geometric, Graphical, ...
- ◆ Use of More Specialist Packages or General Purpose Languages
 - Fortran, C++, CPLEX, GAP, PARI, MAGMA,...
- ◆ Use of Web Applications
 - Sloane's Encyclopedia, Inverse Symbolic Calculator, Fractal Explorer, Euclid in Java, ...
- ◆ Use of Web Databases
 - Google, MathSciNet, Wikipedia, MathWorld, Planet Math, DLMF, MacTutor, Amazon, ...
- ◆ All entail data-mining
 - Clearly the boundaries are blurred and getting blurrier

“Knowing things is very 20th century. You just need to be able to find things.”

- Danny Hillis

- on how Google has already **changed how we think** in [Achenblog](#), July 1 2008

- changing **cognitive styles**

GO

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- Applied Psychological Science
- Awards
- Careers in Psychology
- Decade of Behavior
- Funding
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- Responsible Conduct of Research
- Science Public Policy
- Students
- Testing and Assessment

Interference: The Stroop Effect

Don't read the words on the right--just say the colors they're printed in, and do this aloud as fast as you can.

You're in for a surprise!

If you're like most people, your first inclination was to read the words, 'red, yellow, green...', rather than the colors they're printed in, 'blue, green, red...'

You've just experienced *interference*.

When you look at one of the words, you see both its *color* and its *meaning*. If those two pieces of evidence are in conflict, you have to make a choice. Because experience has taught you that word meaning is more important than ink color, interference occurs when you try to pay attention *only* to the ink color.

The interference effect suggests you're not always in complete control of what you pay attention to.

What do you think would happen:

- If you tried this experiment with a very small child who had not yet learned to read?
- If you tried this experiment with someone who was just learning to speak English?
- If you used the same order of ink colors but wrote non-color words?
- If you made up an experiment of your own.

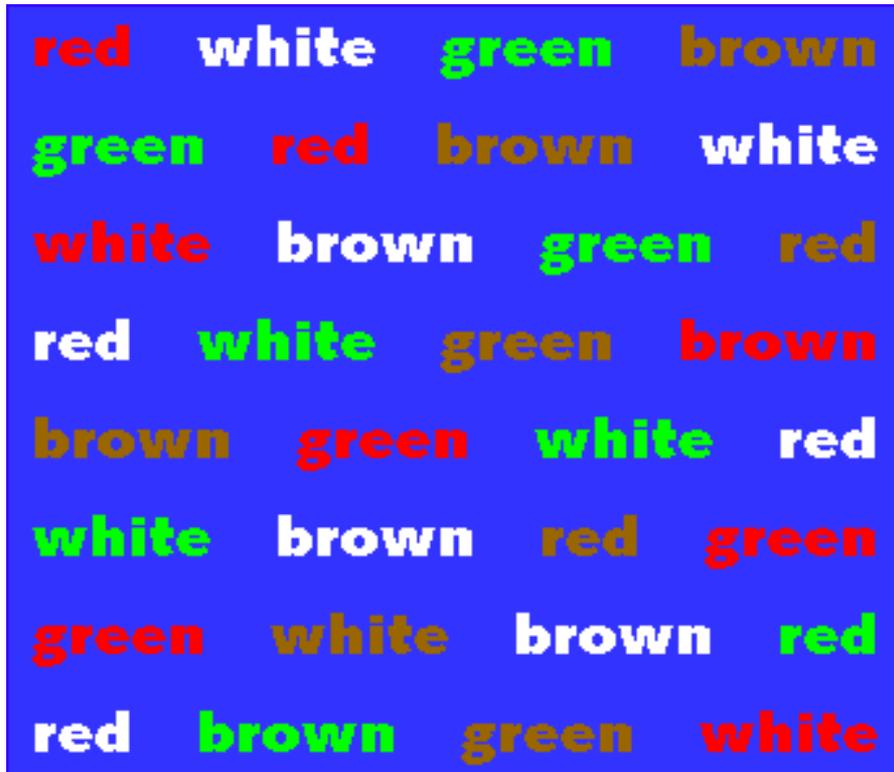
r ed
yellow
green
blue
r ed
blue
yellow
green
blue
r ed

This demonstration is called the Stroop Effect. It is based on the work of Dr. John Ridley Stroop, *Journal of Experimental Psychology*, 1935, and it is part of the museum exhibitions, *PSYCHOLOGY: Understanding Ourselves, Understanding Each Other*, and *PSYCHOLOGY: It's More Than You Think!*, which were developed and produced by the [American Psychological Association](#) and the [Ontario Science Centre](#).



User Experience: Expectations

What is attention? (Stroop test example)



1. Say the color represented by the word.
2. Say the color represented by the font color.

High multitaskers perform # 2 very easily. They are great at suppressing information.

http://www.snre.umich.edu/eplab/demos/st0/stroop_program/stroopgraphicnonshockwave.gif

Acknowledgements: Cliff Nass, CHIME lab, Stanford

The following is a list of useful math tools. The distinction between categories is somewhat arbitrary.

Utilities (General)

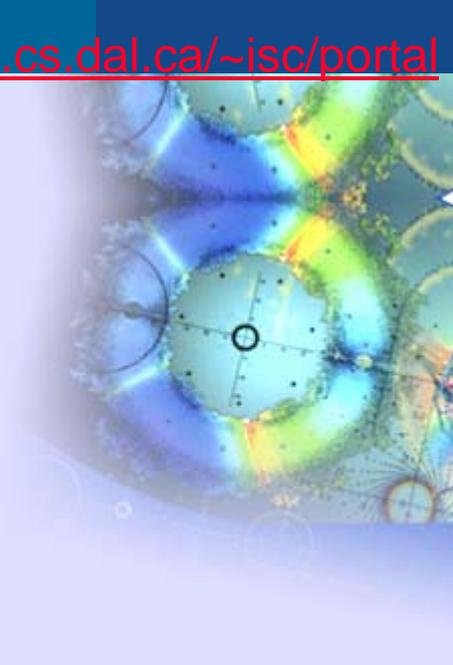
1. [The On-Line Encyclopedia of Integer Sequences](#)
2. [ISC2.0: The Inverse Symbolic Calculator](#)
3. [3D Function Grapher](#)
4. [Julia and Mandelbrot Set Explorer](#)
5. [The KnotPlot Site](#)

Utilities (Special)

6. [EZ Face : Evaluation of Euler Sums and Multiple Zeta Values](#)
7. [GraPHedron: Automated and Computer Assisted Conjectures in Graph Theory](#)
8. [Embree-Trefethen-Wright Pseudospectra and Eigenproblems](#)
9. [Symbolic and Numeric Convex Analysis Tools](#)

Reference

10. [NIST Digital Library of Mathematical Functions\(X\)](#)
11. [Experimental Mathematics Website](#)
12. [Numbers, Constants, and Computation](#)
13. [Numbers: the Competition](#)
14. [The Prime Pages](#)



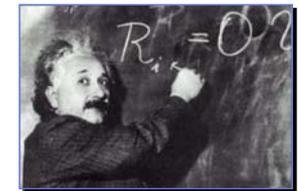
The New Research Landscape (Triangle)

Computational

(dry science)



Experimental
(wet science)



Theoretical
(thought experiments)

The  facilitates
exploratory experimentation
and the use of
wide instrumentation

Exploratory Experiments and Wide Instrumentation

STEINLE goes on to explain that **exploratory experimentation** typically takes place in phases of scientific development **in which no well-formed conceptual framework is available** (Steinle 1997, p. 70). Thus, STEINLE'S exploratory experiments in science are open-ended and highly important and influential in the processes of concept formation.

Drawing on examples from research in molecular biology during the last decades, the philosopher L. R. FRANKLIN adds an interesting dimension to the notion of "exploratory experimentation", namely that of **wide instrumentation**. The availability of high-throughput instruments that can simultaneously measure many features or repeat measurements very quickly has, so FRANKLIN argues, **made it feasible (again) to address the enquiry of nature without local theories to guide the experiments**. In the process, experiments have gained another quality to be measured by, namely efficiency in bringing about new results (Franklin 2005, p. 895).

These aspects of exploratory experimentation and wide instrumentation originate from the philosophy of (natural) science and have not been much developed in the context of experimental mathematics. **However, I claim that e.g. the importance of wide instrumentation for an exploratory approach to experiments that includes concept formation also pertain to mathematics.**"

- H.K. Sørensen, *What's experimental about experimental mathematics?* Preprint, October 2008.

What is Experimental Mathematics?

Chapter 1



What Is Experimental Mathematics?

I know it when I see it.

—Potter Stewart (1915–1985)



What do I see here?

United States Supreme Court justice Potter Stewart famously observed in 1964 that, although he was unable to provide a precise definition of pornography, “I know it when I see it.” We would say the same is true for experimental mathematics. Nevertheless, we realize that we owe our readers at least an approximate initial definition (of experimental mathematics, that is; you’re on your own for pornography) to get started with, and here it is.

Experimental mathematics is the use of a computer to run computations—sometimes no more than trial-and-error tests—to look for patterns, to identify particular numbers and sequences, to gather evidence in support of specific mathematical assertions that may themselves arise by computational means, including search. Like contemporary chemists—and before them the alchemists of old—who mix various substances together in a crucible and heat them to a high temperature to see what happens, today’s experimental mathematician puts a hopefully potent mix of numbers, formulas, and algorithms into a computer in the hope that something of interest emerges.

Experimental Methodology

1. Gaining **insight** and intuition
2. Discovering new relationships
3. **Visualizing** math principles
4. Testing and especially **falsifying conjectures**
5. Exploring a possible result to see **if it merits formal proof**

6. Suggesting approaches for formal proof
7. Computing replacing lengthy hand derivations
8. Confirming analytically derived results

MATH LAB

Computer experiments are transforming mathematics

BY ERICA KLARREICH

Science News
2004

Many people regard mathematics as the crown jewel of the sciences. Yet math has historically lacked one of the defining trappings of science: laboratory equipment. Physicists have their particle accelerators; biologists, their electron microscopes; and astronomers, their telescopes. Mathematics, by contrast, concerns not the physical landscape but an idealized, abstract world. For exploring that world, mathematicians have traditionally had only their intuition.

Now, computers are starting to give mathematicians the lab instrument that they have been missing. Sophisticated software is enabling researchers to travel further and deeper into the mathematical universe. They're calculating the number pi with mind-boggling precision, for instance, or discovering patterns in the contours of beautiful, infinite chains of spheres that arise out of the geometry of knots.

Experiments in the computer lab are leading mathematicians to discoveries and insights that they might never have reached by traditional means. "Pretty much every [mathematical] field has been transformed by it," says Richard Crandall, a mathematician at Reed College in Portland, Ore. "Instead of just being a number-crunching tool, the computer is becoming more like a garden shovel that turns over rocks, and you find things underneath."

At the same time, the new work is raising unsettling questions about how to regard experimental results

"I have some of the excitement that Leonardo of Pisa must have felt when he encountered Arabic arithmetic. It suddenly made certain calculations flabbergastingly easy," Borwein says. "That's what I think is happening with computer experimentation today."

EXPERIMENTERS OF OLD In one sense, math experiments are nothing new. Despite their field's reputation as a purely deductive science, the great mathematicians over the centuries have never limited themselves to formal reasoning and proof.

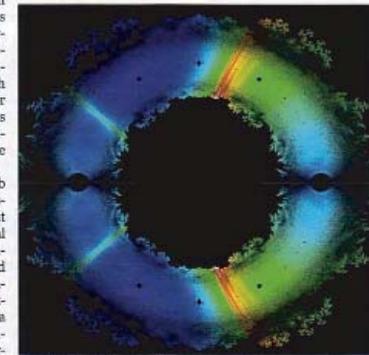
For instance, in 1666, sheer curiosity and love of numbers led Isaac Newton to calculate directly the first 16 digits of the number pi, later writing, "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."

Carl Friedrich Gauss, one of the towering figures of 19th-century mathematics, habitually discovered new mathematical results by experimenting with numbers and looking for patterns. When Gauss was a teenager, for instance, his experiments led him to one of the most important conjectures in the history of number theory: that the number of prime numbers less than a number x is roughly equal to x divided by the logarithm of x .

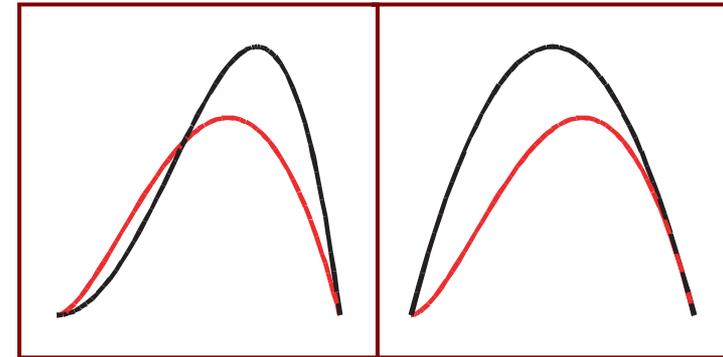
Gauss often discovered results experimentally long before he could prove them formally. Once, he complained, "I have the result, but I do not yet know how to get it."

In the case of the prime number theorem, Gauss later refined his conjecture but never did figure out how to prove it. It took more than a century for mathematicians to come up with a proof.

Like today's mathematicians, math experimenters in the late 19th century used computers—but in those days, the word referred to people with a special facility for calculation.



UNSOLVED MYSTERIES — A computer experiment produced this plot of all the solutions to a collection of simple equations in 2001. Mathematicians are still trying to account for its many features.



Comparing $-y^2 \ln(y)$ (red) to $y-y^2$ and y^2-y^4

Example 1. What's that number? (1995 to 2008)

In **1995** or so Andrew Granville emailed me the number

$$\alpha := 1.433127426722312\dots$$

and challenged me to identify it (our inverse calculator was new in those days).

I asked for its continued fraction? It was

$$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, \dots] \quad (1)$$

I reached for a **good** book on continued fractions and found the answer

$$\alpha = \frac{I_0(2)}{I_1(2)}$$

where I_0 and I_1 are **Bessel functions** of the first kind. (Actually I knew that all arithmetic continued fractions arise in such fashion).

In **2008** there are at least two **or three** other strategies:

- Given (1), type “**arithmetic progression**”, “**continued fraction**” into **Google**
- Type **1,4,3,3,1,2,7,4,2** into **Sloane's Encyclopaedia** of Integer Sequences

I illustrate the results on the next two slides:

“arithmetic progression”, “continued fraction”

In Google on October 15 2008 the first three hits were

Continued Fraction Constant -- from Wolfram MathWorld

- 3 visits - 14/09/07 Perron (1954-57) discusses *continued fractions* having terms even more general than the *arithmetic progression* and relates them to various special functions. ...
mathworld.wolfram.com/ContinuedFractionConstant.html - 31k

HAKMEM -- CONTINUED FRACTIONS -- DRAFT, NOT YET PROOFED

The value of a *continued fraction* with partial quotients increasing in *arithmetic progression* is $I(2/D) A/D [A+D, A+2D, A+3D, \dots]$
www.inwap.com/pdp10/hbaker/hakmem/cf.html - 25k -

On simple continued fractions with partial quotients in arithmetic ...

0. This means that the sequence of partial quotients of the *continued fractions* under investigation consists of finitely many *arithmetic progressions* (with ...
www.springerlink.com/index/C0VXH713662G1815.pdf - by P Bundschuh – 1998

Moreover the [MathWorld](#) entry includes

$$[A + D, A + 2D, A + 3D, \dots] = \frac{I_{A/D}\left(\frac{2}{D}\right)}{I_{1+A/D}\left(\frac{2}{D}\right)}$$

(Schroeppel 1972) for real A and $D \neq 0$.

Example 1: In the Integer Sequence Data Base



Greetings from [The On-Line Encyclopedia of Integer Sequences!](#)

[Hints](#)

Search: 1, 4, 3, 3, 1, 2, 7, 4, 2

Displaying 1-1 of 1 results found.

page

Format: long | [short](#) | [internal](#) | [text](#) Sort: relevance | [references](#) | [number](#) Highlight: on | [off](#)

[A060997](#) Decimal representation of continued fraction 1, 2, 3, 4, 5, 6, 7, ...

1, 4, 3, 3, 1, 2, 7, 4, 2, 6, 7, 2, 2, 3, 1, 1, 7, 5, 8, 3, 1, 7, 1, 8, 3, 4, 5, 5,
7, 7, 5, 9, 9, 1, 8, 2, 0, 4, 3, 1, 5, 1, 2, 7, 6, 7, 9, 0, 5, 9, 8, 0, 5, 2, 3, 4,
3, 4, 4, 2, 8, 6, 3, 6, 3, 9, 4, 3, 0, 9, 1, 8, 3, 2, 5, 4, 1, 7, 2, 9, 0, 0, 1, 3,
6, 5, 0, 3, 7, 2, 6, 4, 3, 5, 7, 8, 6, 1, 1, 4, 6, 5, 9, 5, 0 ([list](#); [cons](#); [graph](#); [listen](#))

OFFSET 1,2

COMMENT The value of this continued fraction is the ratio of two Bessel functions: $\text{BesselI}(0,2)/\text{BesselI}(1,2) = \text{A070910}/\text{A096789}$. Or, equivalently, to the ratio of the sums: $\sum_{n=0..inf} 1/(n!n!)$ and $\sum_{n=0..inf} n/(n!n!)$. - Mark Hudson (mrmarkhudson(AT)hotmail.com), Jan 31 2003

FORMULA $1/\text{A052119}$.

EXAMPLE C=1.433127426722311758317183455775 ...

MATHEMATICA RealDigits[FromContinuedFraction[Range[44]], 10, 110] [[1]]
(* Or *) RealDigits[BesselI[0, 2] / BesselI[1, 2], 10, 110] [[1]]
(* Or *) RealDigits[Sum[1/(n!n!), {n, 0, Infinity}] / Sum[n/(n!n!), {n, 0, Infinity}], 10, 110] [[1]]

CROSSREFS Cf. [A052119](#), [A001053](#).

Adjacent sequences: [A060994](#) [A060995](#) [A060996](#) this_sequence [A060998](#)
[A060999](#) [A061000](#)

Sequence in context: [A016699](#) [A060373](#) [A090280](#) this_sequence [A129624](#)
[A019975](#) [A073871](#)

KEYWORD [cons](#), easy, nonn

AUTHOR Robert G. Wilson v (rgwv(AT)rgwv.com), [May 14 2001](#)

The **Inverse Calculator** returns

Best guess:

BesI(0,2)/BesI(1,2)

- We show the ISC on another number next
- Most functionality of ISC is built into “**identify**” in **Maple**

“The price of metaphor is eternal vigilance.” - Arturo Rosenblueth & Norbert Wiener quoted by R. C. Leowontin, *Science* p.1264, Feb 16, 2001 [[Human Genome Issue](#)].

The inverse Symbolic Calculator (ISC) uses a combination of lookup tables and integer relation algorithms in order to associate with a user-defined, truncated decimal expansion (represented as a floating point expression) a closed form representation for the real number.



The ISC in Action



Standard lookup results for 12.587886229548403854

$\exp(1)+\pi^2$

ISC The original ISC

The Dev Team: Nathan Singer, Andrew Shouldice, Lingyun Ye, Tomas Daske, Peter Dobcsanyi, Dante Manna, O-Yeat Chan, Jon Borwein

3.146264370

19.99909998

ISC The original ISC

The Dev Team: Nathan Singer, Andrew Shouldice, Lingyun Ye, Tomas Daske, Peter Dobcsanyi, Dante Manna, O-Yeat Chan, Jon Borwein

The ISC presently accepts either floating point expressions or correct Maple syntax as input. However, for Maple syntax requiring too long for evaluation, a timeout has been implemented.

Visit

[Jon Borwein's Webpage](#)

[David Bailey's Webpage](#)

[Math Resources Portal](#)

- **ISC+** runs on **Glooscap**
- Less lookup & more algorithms than 1995

Example 2. Pi and 22/7 (Year · through 2008)

The following integral was made popular in a 1971 **Eureka** article

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

- Set on a 1960 Sydney honours final, it perhaps originated in 1941 with Dalziel (author of the 1971 article who did not reference himself)!

Why trust the evaluation? Well Maple and Mathematica both 'do it'

- A better answer is to ask **Maple** for

$$\int_0^t \frac{(1-x)^4 x^4}{1+x^2} dx$$

- It will return

$$\int_0^t \frac{x^4 (1-x)^4}{1+x^2} dx = \frac{1}{7} t^7 - \frac{2}{3} t^6 + t^5 - \frac{4}{3} t^3 + 4t - 4 \arctan(t)$$

and now differentiation and the **Fundamental theorem of calculus** proves the result.

- **Not a conventional proof** but a totally rigorous one. (An 'instrumental use' of the computer)

Example 3: Multivariate Zeta Values

In **1993**, Enrico Au-Yeung, then an undergraduate in Waterloo, came into my office and asserted that:

$$\sum_{k=1}^{\infty} \left(1 + \frac{1}{2} + \cdots + \frac{1}{k}\right)^2 k^{-2} = 4.59987\dots \approx \frac{17}{4}\zeta(4) = \frac{17\pi^4}{360}$$

I was very skeptical, but **Parseval's identity** computations affirmed this to high precision. This is reducible to a case of the following class:

$$\zeta(s_1, s_2, \dots, s_k) = \sum_{n_1 > n_2 > \dots > n_k > 0} \prod_{j=1}^k n_j^{-|s_j|} \sigma_j^{-n_j},$$

where s_j are integers and $\sigma_j = \text{signum } s_j$. These can be rapidly computed using a scheme implemented in an online tool:

www.cecm.sfu.ca/projects/ezface+. They have become of more and more interest in number theory, combinatorics, knot theory and mathematical physics. A marvellous example is **Zagier's** (now proven) **conjecture**

$$\frac{17}{360} = 0.47222\dots$$

$$\zeta\left(\overbrace{3, 1, 3, 1, \dots, 3, 1}^n\right) = \frac{2\pi^{4n}}{(4n+2)!}$$

Example 3. Related Matrices (1993-2006)

In the course of proving conjectures about **multiple zeta values** we needed to obtain the closed form partial fraction decomposition for

$$\frac{1}{x^s(1-x)^t} = \sum_{j \geq 0} \frac{a_j^{s,t}}{x^j} + \sum_{j \geq 0} \frac{b_j^{s,t}}{(1-x)^j} \quad a_j^{s,t} = \binom{s+t-j-1}{s-j}$$

This was known to Euler but is easily discovered in **Maple**. We needed also to show that **M=A+B-C** was invertible where the n by n matrices A, B, C respectively had entries

$$(-1)^{k+1} \binom{2n-j}{2n-k}, \quad (-1)^{k+1} \binom{2n-j}{k-1}, \quad (-1)^{k+1} \binom{j-1}{k-1}$$

Thus, A and C are triangular and B is full. After messing around with lots of cases it occurred to me to ask for the **minimal polynomial** of M

$$> \text{linalg}[\text{minpoly}](M(12),t); \quad -2 + t + t^2$$

$$> \text{linalg}[\text{minpoly}](B(20),t); \quad -1 + t^3$$

$$> \text{linalg}[\text{minpoly}](A(20),t); \quad -1 + t^2$$

$$> \text{linalg}[\text{minpoly}](C(20),t); \quad -1 + t^2$$

$$M(6) = \begin{bmatrix} 1 & -22 & 110 & -330 & 660 & -924 \\ 0 & -10 & 55 & -165 & 330 & -462 \\ 0 & -7 & 36 & -93 & 162 & -210 \\ 0 & -5 & 25 & -56 & 78 & -84 \\ 0 & -3 & 15 & -31 & 35 & -28 \\ 0 & -1 & 5 & -10 & 10 & -6 \end{bmatrix}$$

Example 3. The Matrices Conquered

Once this was discovered proving that for all $n > 2$

$$A^2 = I, \quad BC = A, \quad C^2 = I, \quad CA = B^2$$

is a nice combinatorial exercise (by hand or computer). Clearly then

$$B^3 = B \cdot B^2 = B(CA) = (BC)A = A^2 = I$$

and the formula

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

is again a fun exercise in formal algebra; as is confirming that we have discovered an amusing representation of the symmetric group S_3 .

- characteristic or minimal polynomials (rather abstract for me as a student) now become members of a rapidly growing box of symbolic tools, as do many **matrix decompositions**, **Groebner bases** etc ...
- a **typical** matrix has a full degree minimal polynomial

Example 4. Numerical Integration (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 these (now proven) **arithmetic** results:

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

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

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

Example 4: Identifying the Limit Using the Inverse Symbolic Calculator (2.0)

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

$$C_{1024} = 0.630473503374386796122040192710878904354587\dots$$

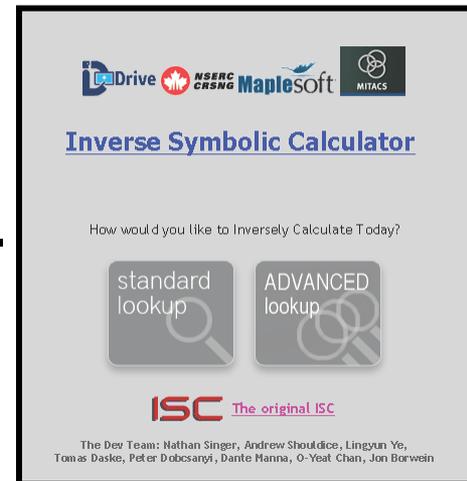
We then used the Inverse Symbolic Calculator, the online numerical constant recognition facility available at:

<http://ddrive.cs.dal.ca/~isc/portal>

Output: Mixed constants, 2 with elementary transforms.
 $.6304735033743867 = \text{sr}(2)^2 / \exp(\gamma)^2$

In other words,

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

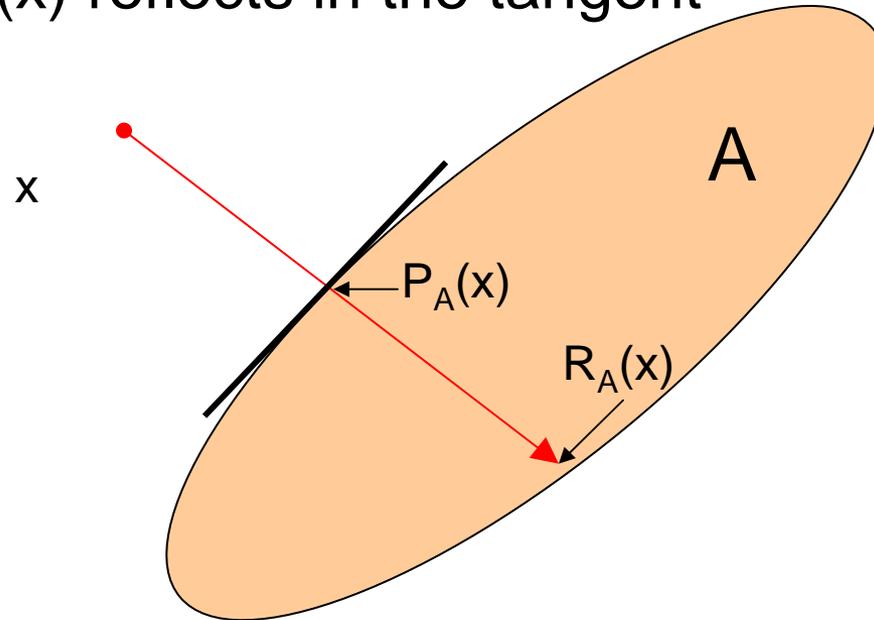


References. Bailey, Borwein and Crandall, "Integrals of the Ising Class," *J. Phys. A.*, **39** (2006)

Bailey, Borwein, Broadhurst and Glasser, "Elliptic integral representation of Bessel moments," *J. Phys. A*, **41** (2008) [IoP Select]

Example 5: A Simple Phase Reconstruction Model

Projectors and Reflectors: $P_A(x)$ is the metric projection or nearest point and $R_A(x)$ reflects in the tangent



In the convex case to find $x \in A \cap B$ the *method of alternating projections*

$$y_n := P_B(x_n), \quad x_{n+1} := P_A(y_n)$$

works very well and parallelizes to products of sets (used on Hubble)

Example 5: Phase Reconstruction

In a wide variety of problems (protein folding, 3SAT, Sudoku) B is non-convex but “divide and concur” works better than theory can explain. It is:

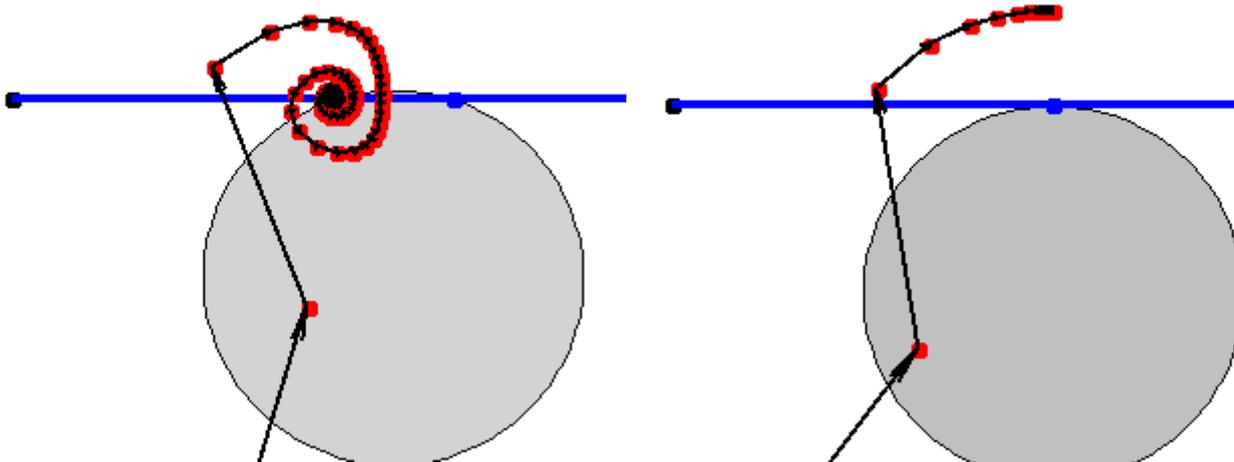
$$R_A(x) := 2P_A(x) - x \text{ and } x \rightarrow \frac{x + R_A(R_B(x))}{2}$$

Consider the **simplest case** of a line A of height α and the unit circle B.

With $z_n := (x_n, y_n)$ the iteration becomes

$$x_{n+1} := \cos \theta_n, y_{n+1} := y_n + \alpha - \sin \theta_n, \quad (\theta_n := \arg z_n)$$

For $\alpha=0$ proven convergence to one of the two points in $A \cap B$ iff start off vertical axis. For $\alpha>1$ (infeasible) iterates go vertically to infinity. For $\alpha=1$ (tangent) iterates converge to point above tangent. For $\alpha \in (0,1)$ the pictures are lovely but proofs escape me. *Maple* (Cinderella) pictures follow:



An ideal problem to introduce early under-graduates to research, with many accessible extensions in 2 or 3 dimensions

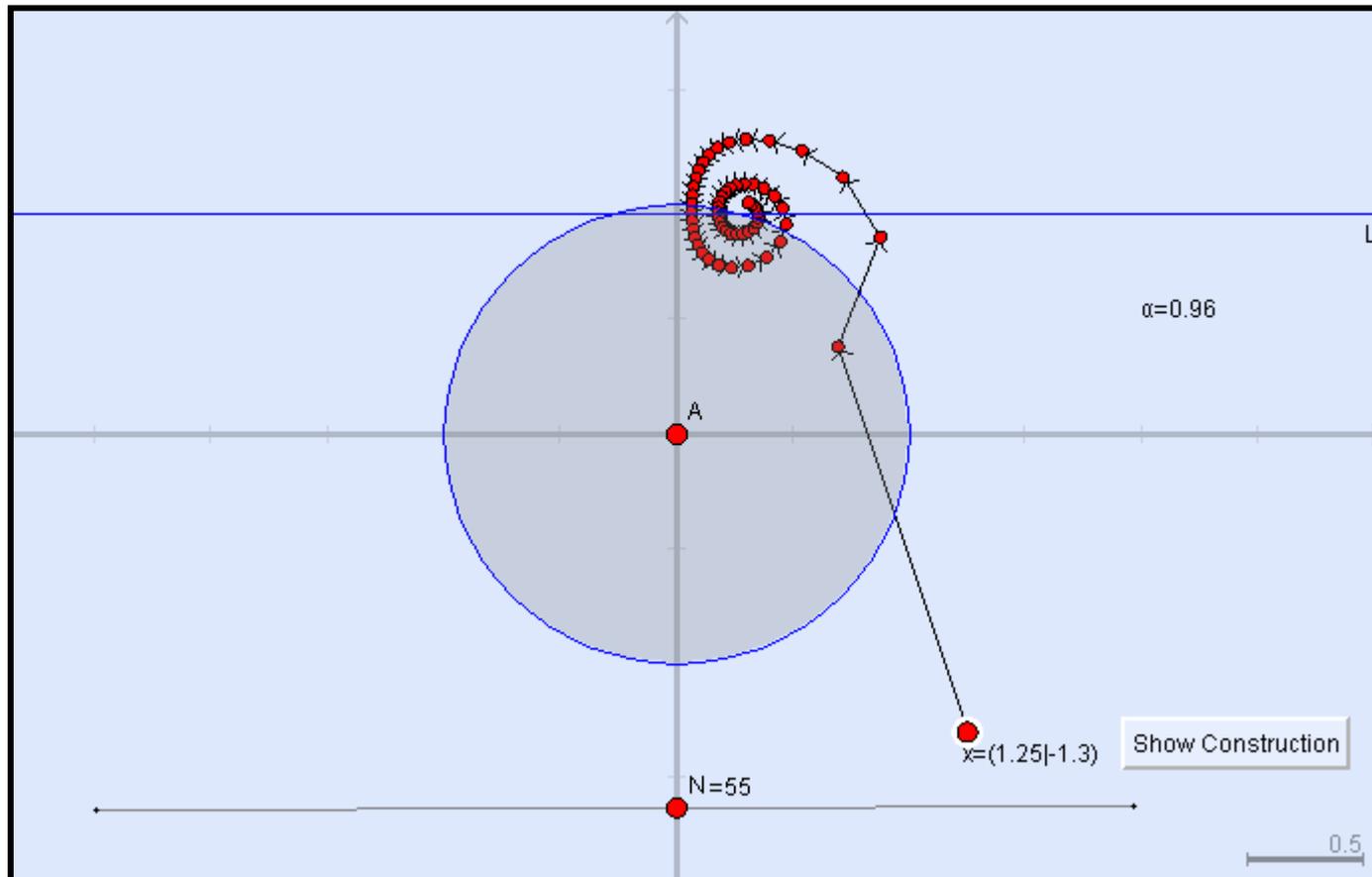
Dynamic Phase Reconstruction in Cinderella

Consider the **simplest case** of a line A of height α and the unit circle B.

With $z_n := (x_n, y_n)$ the iteration becomes

$$x_{n+1} := \cos \theta_n, y_{n+1} := y_n + \alpha - \sin \theta_n, \quad (\theta_n := \arg z_n)$$

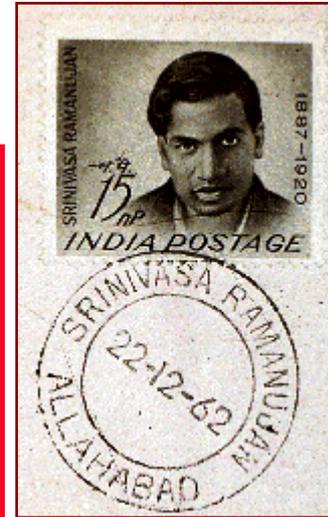
For $\alpha \in (0,1)$ the pictures are lovely but proofs escape me. A *Cinderella* picture follows:



A Sidebar: New Ramanujan-Like Identities

Guillera has recently 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

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

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 proof.** It seems there are no higher-order analogues.

“Why should I refuse a good dinner simply because I don't understand the digestive processes involved?” - Oliver Heaviside (1850-1925) **when criticized for daring to use his operators before they could be justified formally**

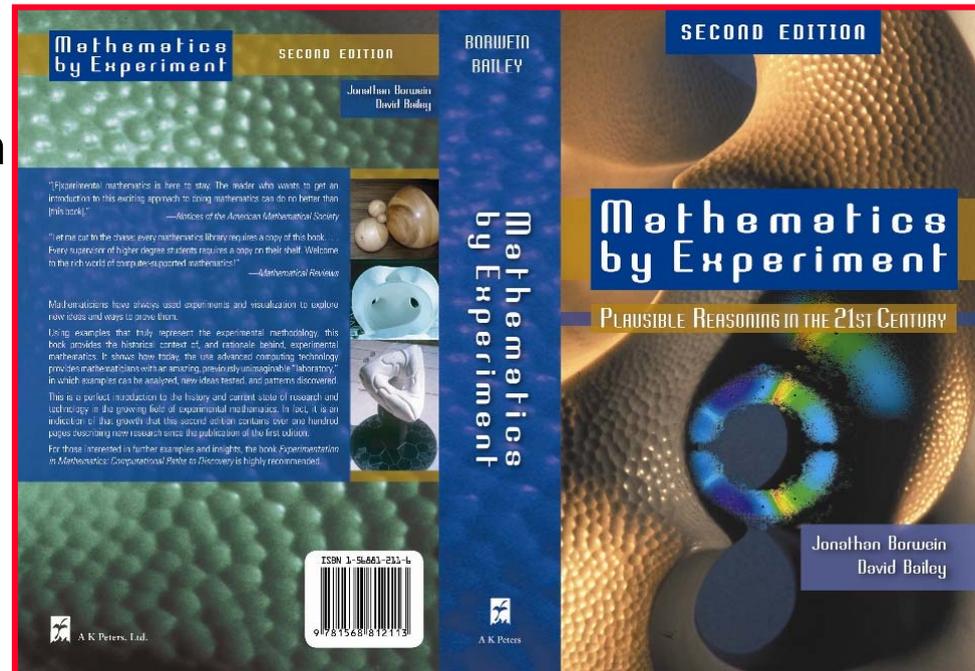
First Conclusions

- ◆ The students of **2010** live in an information-rich, judgement-poor world
- ◆ The explosion of information is not going to diminish
- ◆ So we have to teach judgement (**not obsessive concern with plagiarism**)
 - that means mastering the sorts of tools I have illustrated
- ◆ We also have to acknowledge that most of our classes will contain a very broad variety of skills and interests (**few future mathematicians**)
 - properly balanced, discovery and proof can live side-by-side and allow for the mediocre and the talented to flourish in their own fashion
- ◆ **Impediments** to the assimilation of the tools I have illustrated are myriad (**as I am only too aware from recent teaching experiences**)
- ◆ These impediments include our own inertia and
 - organizational and technical bottlenecks (IT - **not so much dollars**)
 - under-prepared or mis-prepared colleagues
 - the dearth of good material from which to teach a modern syllabus

"The plural of 'anecdote' is not 'evidence'."
- Alan L. Leshner, *Science's* publisher

Further Conclusions

- ◆ New techniques now permit integrals, infinite series sums and other entities to be evaluated to high precision (hundreds or thousands of digits), thus permitting PSLQ-based schemes to discover new identities.
- ◆ These methods typically do not suggest proofs, but often it is much easier to find a proof (say via WZ) when one “knows” the answer is right.

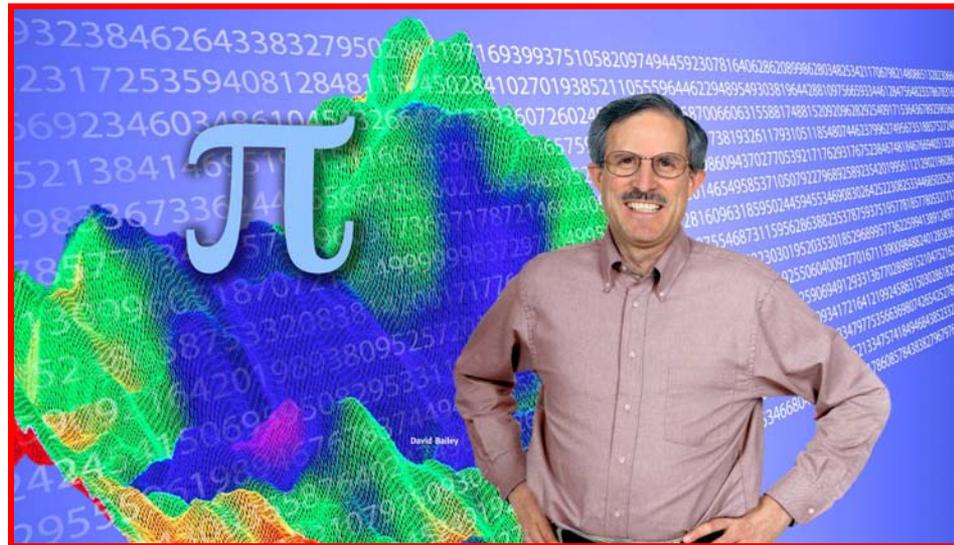


For more details of the examples see *Mathematics by Experiment* (2003-08), *Experimentation in Mathematics* (2004) with Roland Girgensohn, or *Experimental Mathematics in Action* (2007). A “Reader’s Digest” version of the first two is at www.experimentalmath.info with much other material.

“The future has arrived; it's just not evenly distributed.” - Douglas Gibson (who coined the term ‘cyberspace’)

Three Extra Examples

1. Zeta Values and PSLQ
2. Reciprocal Series for π and Wilf-Zeilberger
3. A Cautionary Example



David Bailey on the side of a Berkeley bus

“Anyone who is not shocked by quantum theory has not understood a single word.” - Niels Bohr

Example: Apéry-Like Summations

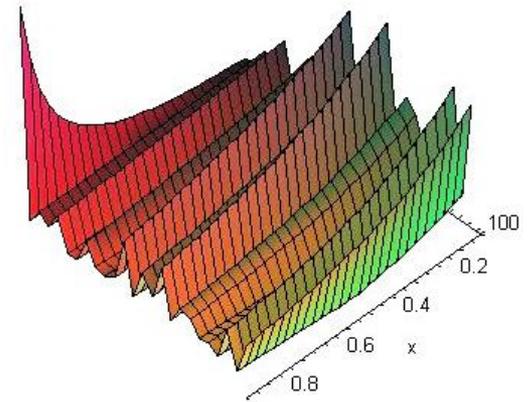
The following formulas for $\zeta(n)$ have been known for many decades:

$$\zeta(2) = 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k}}, \text{ (known to Euler?)}$$

$$\zeta(3) = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}}, \text{ (Apéry, 1979)}$$

$$\zeta(4) = \frac{36}{17} \sum_{k=1}^{\infty} \frac{1}{k^4 \binom{2k}{k}}, \text{ (Comtet, 1974).}$$

The RH in Maple



These results have a unified proof (BBK 2001) and have led many to hope 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 shown that if Q_5 satisfies a polynomial with **degree** at most **25**, then at least **one coefficient** has **380** digits.

Apéry II: Nothing New under the Sun

Margo Kondratieva found a formula of Markov in 1890:

$$\sum_{n=1}^{\infty} \frac{1}{(n+a)^3} = \frac{1}{4} \sum_{n=0}^{\infty} \frac{(-1)^n (n!)^6}{(2n+1)!} \times \frac{(5(n+1)^2 + 6(a-1)(n+1) + 2(a-1)^2)}{\prod_{k=0}^n (a+k)^4}.$$

Note: *Maple* establishes this identity as

$$-1/2 \Psi(2, a) = -1/2 \Psi(2, a) - \zeta(3) + 5/4 {}_4F_3([1, 1, 1, 1], [3/2, 2, 2], -1/4)$$

Hence

$$\zeta(4) = - \sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{\binom{2m}{m} m^4} + \frac{10}{3} \sum_{m=1}^{\infty} \frac{(-1)^{m-1} \sum_{k=1}^m \frac{1}{k}}{\binom{2m}{m} m^3}.$$

- ◆ The case $a=0$ is the formula used by Apéry his **1979** proof that $\zeta(3) \notin \mathbb{Q}$

“How extremely stupid not to have thought of that!” - Thomas Henry Huxley (1825-1895) ‘Darwin's Bulldog’ was initially unconvinced of evolution.

Example: Use of the Wilf-Zeilberger Method

As noted two post **2000** experimentally-discovered identities are

$$\sum_{n=0}^{\infty} \frac{\binom{4n}{2n} \binom{2n}{n}^4}{2^{16n}} (120n^2 + 34n + 3) = \frac{32}{\pi^2}$$

$$\sum_{n=0}^{\infty} \frac{(-1)^n \binom{2n}{n}^5}{2^{20n}} (820n^2 + 180n + 13) = \frac{128}{\pi^2}$$

To effect a proof Guillera 'cunningly' started by defining

$$G(n, k) = \frac{(-1)^k}{2^{16n} 2^{4k}} (120n^2 + 84nk + 34n + 10k + 3) \frac{\binom{2n}{n}^4 \binom{2k}{k}^3 \binom{4n-2k}{2n-k}}{\binom{2n}{k} \binom{n+k}{n}^2}$$

He then used the **EKHAD** software package to obtain the companion

$$F(n, k) = \frac{(-1)^k 512}{2^{16n} 2^{4k}} \frac{n^3}{4n - 2k - 1} \frac{\binom{2n}{n}^4 \binom{2k}{k}^3 \binom{4n-2k}{2n-k}}{\binom{2n}{k} \binom{n+k}{n}^2}$$

Example Usage of W-Z, II

When we define

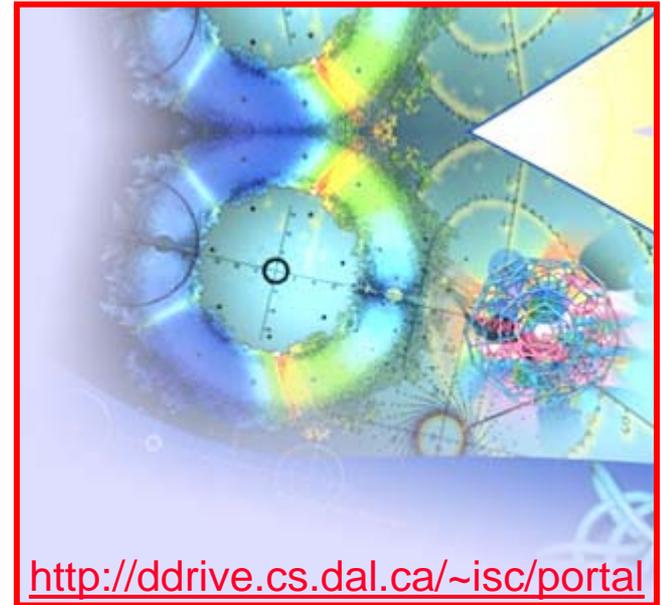
$$H(n, k) = F(n + 1, n + k) + G(n, n + k)$$

Zeilberger's theorem gives the identity

$$\sum_{n=0}^{\infty} G(n, 0) = \sum_{n=0}^{\infty} H(n, 0)$$

which when written out is

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4 \binom{4n}{2n}}{2^{16n}} (120n^2 + 34n + 3) &= \sum_{n=0}^{\infty} \frac{(-1)^n (n+1)^3 \binom{2n+2}{n+1}^4 \binom{2n}{n}^3 \binom{2n+4}{n+2}}{2^{20n+7} (2n+3) \binom{2n+2}{n} \binom{2n+1}{n+1}^2} \\ &+ \sum_{n=0}^{\infty} \frac{(-1)^n}{2^{20n}} (204n^2 + 44n + 3) \binom{2n}{n}^5 = \frac{1}{4} \sum_{n=0}^{\infty} \frac{(-1)^n \binom{2n}{n}^5}{2^{20n}} (820n^2 + 180n + 13) \end{aligned}$$



<http://ddrive.cs.dal.ca/~isc/portal>

A limit argument completes the proof of Guillera's identities.

A Cautionary Example

These **constants agree to 42 decimal digits** accuracy, but are **NOT** equal:

$$\int_0^{\infty} \cos(2x) \prod_{n=1}^{\infty} \cos(x/n) dx =$$

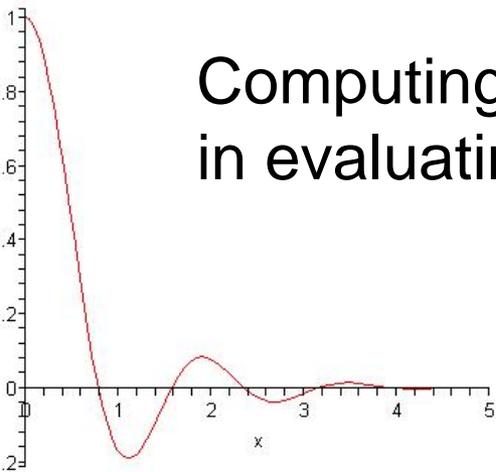
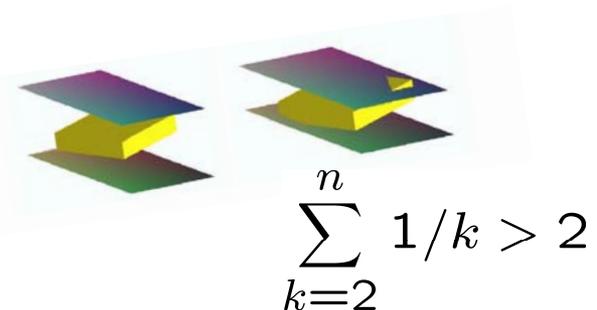
0.39269908169872415480783042290993786052464543418723...

$$\frac{\pi}{8} =$$

0.39269908169872415480783042290993786052464617492189...

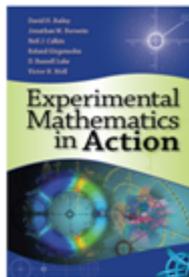
Computing this integral is nontrivial, due largely to difficulty in evaluating the integrand function to high precision.

Fourier transforms **turn the integrals into volumes** and neatly explains **this happens when a hyperplane meets a hypercube (LP) ...**



Experimental Mathematics in Action

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



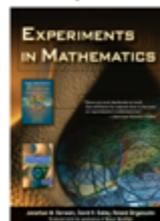
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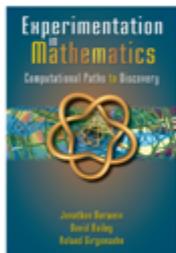


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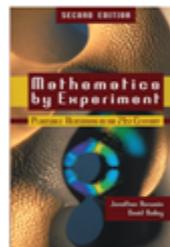
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