Computational Paths to Mathematical Discovery

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Computers in Mathematics

Although the computer's origin was in the field of pure mathematics, computer technology has heretofore played a relatively minor role in mathematical research.

A sea change is now underway:

- Powerful, broad-spectrum mathematical computing software, especially Mathematica and Maple.
- High-precision computation facilities.
- Useful Internet-based tools, particularly for sequence and constant recognition.
- Advanced visualization tools.

A new generation of mathematicians, raised in the computer age, is eagerly using these new tools, and a wave of new discoveries are being made.

The Experimental Methodology in Mathematics

- Gaining insight and intuition.
- Discovering new patterns and relationships.
- Using graphical displays to suggest underlying mathematical principles.
- Testing and especially falsifying conjectures.
- Exploring a possible result to see if it is worth formal proof.
- Suggesting approaches for formal proof.
- Replacing lengthy hand derivations with computer-based derivations.
- Confirming analytically derived results.

Mathematica and Maple

Due to in part to fierce competition, both now feature a formidable array of advanced features:

- Multi-variable symbolic manipulation – can work with expressions involving literally millions of terms.
- Hundreds of elementary and advanced functions.
- Powerful symbolic integration and differentiation.
- Summation of infinite series.
- High-precision numerical evaluation of virtually all defined functions.
- 2-D and 3-D plotting.

Mathematica In Action

```
In[1]: Sum[1/16^k*(4/(8*k+1) - 2/(8*k+4) - 1/(8*k+5) \
       - 1/(8*k+6)), {k, 0, Infinity}]

Out[1]: -2 ArcTanh[1/4] + 4 Hypergeometric2F1[1, 1/8, 9/8, 1/16]
   - 1/5 Hypergeometric2F1[1, 5/8, 13/8, 1/16]
   - 1/6 Hypergeometric2F1[1, 3/4, 7/4, 1/16]

In[2]: FullSimplify[%]

Out[2]: π
```

Neil Sloane's Online Dictionary of Integer Sequences

Available at: **http://www.research.att.com/~njas/sequences**

Example of usage:

[Input:] `1, 2, 3, 6, 11, 23, 47, 106, 235`

[Output:]

```
ID Number: A000364 (Formerly M4019 and N1667)
URL: http://www.research.att.com/projects/OEIS?Anum=A000364
   Sequence:
   1,1,5,61,1385,50521,2702765,199360981,19391512145,
   2404879675441,370371188237525,69348874393137901, […]
Name: Euler (or secant or "Zig") numbers: expansion of sec x.
References M. Abramowitz and I. A. Stegun, eds., Handbook of
   Mathematical Functions, National Bureau of Standards
   Applied Math. Series 55, 1964 (and various reprintings), p.
   810; gives a version with signs: E_{2n} = (-1)^n*a(n).
[and additional information]
```

The CECM On-Line Inverse Symbolic Calculator

Available at: **http://www.cecm.sfu.ca/projects/ISC**

Example of usage:

[Input:]

`0.5805649647699622716961465294044794`

[Output:]

```
K satisfies the following Z-linear combination :
    - 17 K + Pi**2
```

In other words, input constant is probably $\pi^2/17$.

LBNL's Arbitrary Precision Computation (ARPREC) Package

- Low-level routines written in C++.
- C++ and F-90 translation modules permit use with existing programs with only minor code changes.
- Double-double (32 digits), quad-double, (64 digits) and arbitrary precision (>64 digits) available.
- Special routines for extra-high precision (>1000 dig).
- Includes common math functions: sqrt, cos, exp, etc.
- PSLQ, root finding, numerical integration.
- An interactive "Experimental Mathematician's Toolkit" employing this software is also available.

Available at: **http://www.expmath.info**

The PSLQ Integer Relation Algorithm

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

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

- At the present time, the PSLQ algorithm of Helaman Ferguson is the best algorithm for integer relation detection.
- PSLQ was named one of ten "algorithms of the century" by *Computing in Science and Engineering*.
- High precision arithmetic software is required:

  At least d x n digits, where d is the size (in digits) of the largest of the integers a_k.

Ferguson's "Eight-Fold Way" Sculpture

Application of PSLQ: Bifurcation Points in Chaos Theory

B_3 = 3.54409035955… is third bifurcation point of the logistic iteration of chaos theory:

$$x_{n+1} = r x_n (1 - x_n)$$

i.e., B_3 is the smallest r such that the iteration exhibits 8-way periodicity instead of 4-way periodicity.

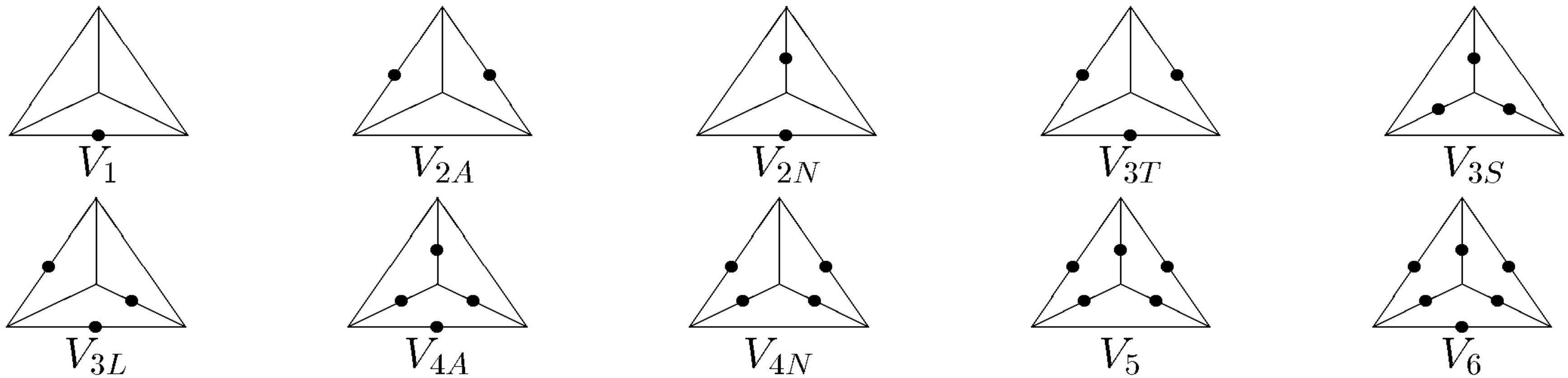
In 1990, a predecessor to PSLQ found that B_3 is a root of the polynomial

$$0 = 4913 + 2108t^2 - 604t^3 - 977t^4 + 8t^5 + 44t^6 + 392t^7 - 193t^8 - 40t^9 + 48t^{10} - 12t^{11} + t^{12}$$

Recently B_4 was identified as the root of a 256-degree polynomial by a much more challenging computation.

These results have subsequently been proven formally.

Evaluation of Ten Constants from Quantum Field Theory



$$
\begin{aligned}
V_1 &= 6\zeta(3) + 3\zeta(4) \\
V_{2A} &= 6\zeta(3) - 5\zeta(4) \\
V_{2N} &= 6\zeta(3) - \frac{13}{2}\zeta(4) - 8U \\
V_{3T} &= 6\zeta(3) - 9\zeta(4) \\
V_{3S} &= 6\zeta(3) - \frac{11}{2}\zeta(4) - 4C^2 \\
V_{3L} &= 6\zeta(3) - \frac{15}{4}\zeta(4) - 6C^2 \\
V_{4A} &= 6\zeta(3) - \frac{77}{12}\zeta(4) - 6C^2 \\
V_{4N} &= 6\zeta(3) - 14\zeta(4) - 16U
\end{aligned}
$$

$$
\begin{aligned}
V_5 &= 6\zeta(3) - \frac{469}{27}\zeta(4) + \frac{8}{3}C^2 - 16V \\
V_6 &= 6\zeta(3) - 13\zeta(4) - 8U - 4C^2
\end{aligned}
$$

where

$$
\begin{aligned}
C &= \sum_{k>0} \sin(\pi k/3)/k^2 \\
U &= \sum_{j>k>0} \frac{(-1)^{j+k}}{j^3 k} \\
V &= \sum_{j>k>0} (-1)^j \cos(2\pi k/3)/(j^3 k)
\end{aligned}
$$

Numerical Integration and the Euler-Maclaurin Formula

Suppose f(x) is at least 2m-times continuously differentiable. Given n, let h = (b - a)/n and x_j = a + j h). Then

$$\int_a^b f(x)\,dx = h \sum_{j=0}^{n} f(x_j) - \frac{h}{2}(f(a) + f(b)) - \sum_{i=1}^{m} \frac{h^{2i} B_{2i}}{(2i)!}\left(f^{(2i-1)}(b) - f^{(2i-1)}(a)\right) - E$$

$$E = \frac{h^{2m+2}(b-a) B_{2m+2} f^{2m+2}(\xi)}{(2m+2)!}$$

Conclusion: For certain smooth, bell-shaped functions, where f(t) and all of its derivatives are zero at a and b, a simple block-function approximation to the integral is remarkably accurate – the error E goes to zero more rapidly than any power of the interval h.

Same conclusion applies for integrals on (-infinity, infinity).

New Quadrature Methods Based on the E-M Formula

Given f(x) defined on (-1,1), we employ a function g(t) such that g(t) goes from -1 to 1 over the real line, with g'(t) going to zero for large |t|. Then

$$\int_{-1}^{1} f(x)\,dx \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\,dt \;\approx\; h\sum_{-\infty}^{\infty} w_j f(x_j)$$

where $x_j = g(hj)$ and $w_j = g'(hj)$. For "erf" quadrature,

$$g(t) \;=\; \mathrm{erf}(t) \qquad g'(t) \;=\; \frac{2}{\sqrt{\pi}} e^{-t^2}$$

For "tanh-sinh" quadrature,

$$g(t) \;=\; \tanh(\pi/2\cdot\sinh t) \qquad g'(t) \;=\; \frac{\pi/2\cdot\sinh t}{\cosh^2(\pi/2\cdot\sinh t)}$$

Example of Erf Quadrature

Example problem (note blow-up singularity at π/2):

$$\int_0^{\pi/2} \sqrt{\tan t}\, dt \;=\; \pi\sqrt{2}/2$$

Accuracy of erf quadrature at successive levels:

Level	h	Evaluations	Accuracy
1	2	16	10^{-1}
2	1	32	10^{-3}
3	2^{-1}	64	10^{-8}
4	2^{-2}	128	10^{-16}
5	2^{-3}	256	10^{-33}
6	2^{-4}	512	10^{-66}
7	2^{-8}	1024	10^{-132}
8	2^{-16}	2048	10^{-264}
9	2^{-32}	4096	10^{-527}
10	2^{-64}	8192	10^{-1001}

A Quadrature-PSLQ Result

Using a high-precision quadrature program, together with PSLQ, Jon Borwein and I found that if

$$C(a) = \int_0^1 \frac{\arctan \sqrt{x^2 + a^2}}{(x^2 + 1)\sqrt{x^2 + a^2}} dx$$

Then

$$\begin{aligned} C(0) &= (\pi \log 2)/8 + G/2 \\ C(1) &= \pi/4 - \pi\sqrt{2}/2 + 3\sqrt{2}/2 \cdot \arctan \sqrt{2} \\ C(\sqrt{2}) &= 5\pi^2/96 \end{aligned}$$

Several general results have also been found.

Another Quadrature-PSLQ Result

$$\frac{2}{\sqrt{3}}\int_0^1 \frac{\log^6(x)\arctan[x\sqrt{3}/(x-2)]}{x+1}\,dx \;=\; \frac{1}{81648}\Big(-229635L_3(8)+29852550L_3(7)\log 3$$
$$-1632960L_3(6)\pi^2+27760320L_3(5)\zeta(3)$$
$$-275184L_3(4)\pi^4+36288000L_3(3)\zeta(5)$$
$$-30008L_3(2)\pi^6-57030120L_3(1)\zeta(7)\Big),$$

where

$$L_3(s) \;=\; \sum_{n=1}^{\infty}\left(1/(3n-2)^s-1/(3n-1)^s\right)$$

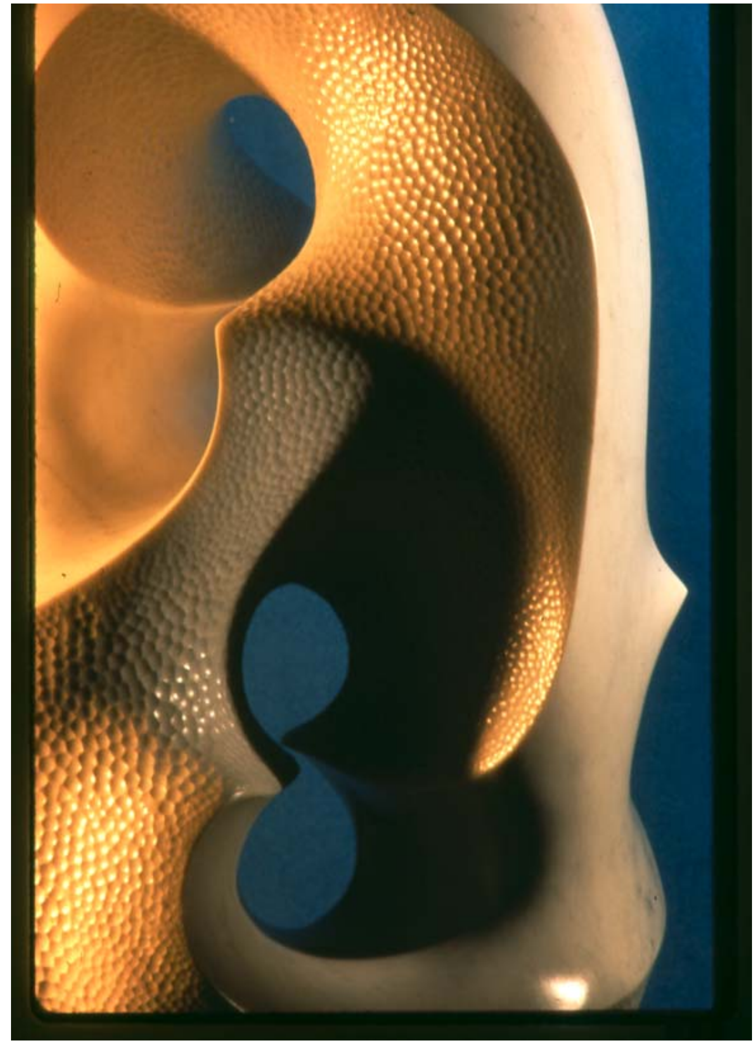
PSLQ and Sculpture

The complement of the figure-eight knot, when viewed in hyperbolic space, has finite volume

V = 2.02988321281930725004…

Recently David Broadhurst found, using PSLQ, that V is given by the formula:

$$V = \frac{\sqrt{3}}{9} \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n} \left(\frac{18}{(6n+1)^2} - \frac{18}{(6n+2)^2} - \frac{24}{(6n+3)^2} - \frac{6}{(6n+4)^2} + \frac{2}{(6n+5)^2} \right)$$



Some Supercomputer-Class PSLQ Solutions

- Identification of B_4, the fourth bifurcation point of the logistic iteration.
  - Integer relation of size 121; 10,000 digit arithmetic.
- Identification of Apery sums.
  - 15 integer relation problems, with size up to 118, requiring up to 5,000 digit arithmetic.
- Identification of Euler-zeta sums.
  - Hundreds of integer relation problems, each of size 145 and requiring 5,000 digit arithmetic.
  - Run on IBM SP parallel system.
- Finding relation involving root of Lehmer's polynomial.
  - Integer relation of size 125; 50,000 digit arithmetic.
  - Utilizes 3-level, multi-pair parallel PSLQ program.
  - Run on IBM SP using ARPEC; 16 hours on 64 CPUs.

Cautionary Example #1

$$\int_0^\infty \frac{\sin x}{x} dx = \frac{\pi}{2}$$

$$\int_0^\infty \frac{\sin x}{x} \cdot \frac{\sin(x/3)}{x/3} dx = \frac{\pi}{2}$$

$$\int_0^\infty \frac{\sin x}{x} \cdot \frac{\sin(x/3)}{x/3} \cdot \frac{\sin(x/5)}{x/5} dx = \frac{\pi}{2}$$

$$\cdots$$

$$\int_0^\infty \frac{\sin x}{x} \cdot \frac{\sin(x/3)}{x/3} \cdot \frac{\sin(x/5)}{x/5} \cdots \frac{\sin(x/13)}{x/13} dx = \frac{\pi}{2}$$

but

$$\int_0^\infty \frac{\sin x}{x} \cdot \frac{\sin(x/3)}{x/3} \cdot \frac{\sin(x/5)}{x/5} \cdots \frac{\sin(x/15)}{x/15} dx$$

$$= \frac{467807924713440738696537864469}{935615849440640907310521750000} \pi$$

Cautionary Example #2

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

$$\int_0^\infty \cos(2x) \prod_{n=0}^{\infty} \cos(x/n)\, dx \quad =$$

$$0.392699081698724154807830422909937860524645434187231\ldots$$

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

$$0.392699081698724154807830422909937860524646174921888\ldots$$

Fascination With Pi

Newton (1670):

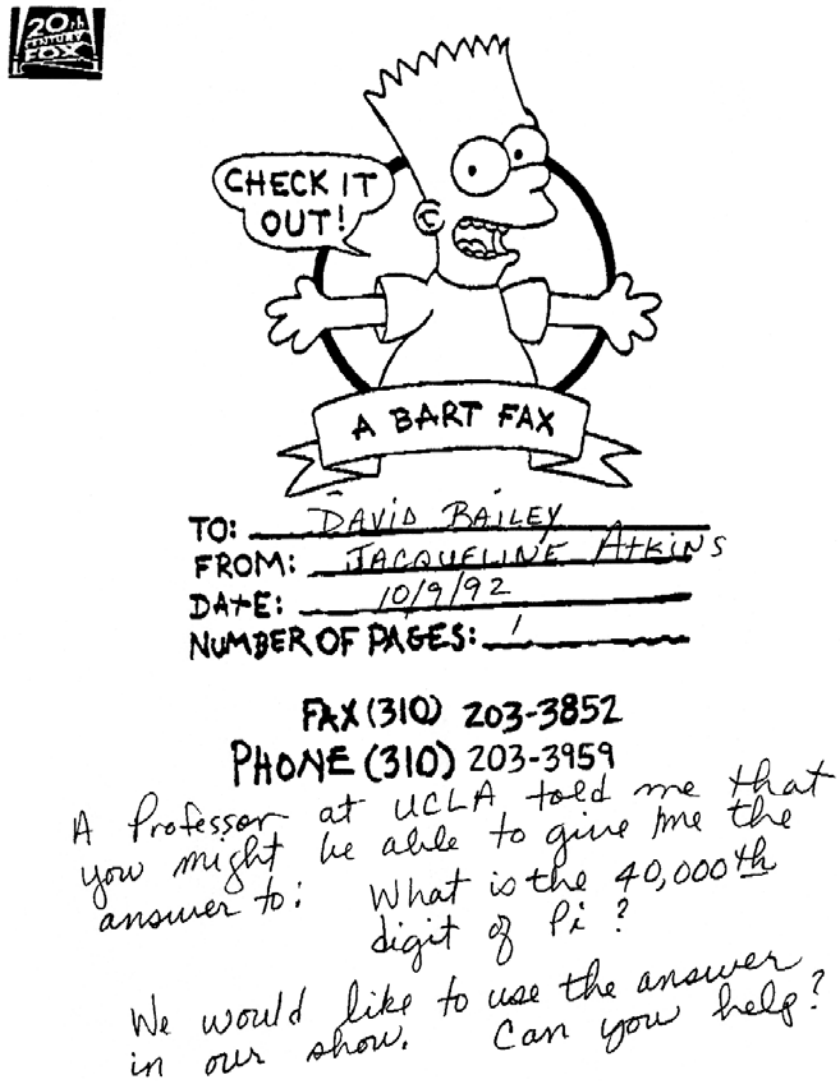
- "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."

Carl Sagan (1986):

- In his book "Contact," the lead scientist (played by Jodie Foster in the movie) looked for patterns in the digits of pi.

Carl E. Sagan

Fax from “The Simpsons” Show



20th Century Fox

CHECK IT OUT!

A BART FAX

TO: DAVID BAILEY

FROM: JACQUELINE ATKINS

DATE: 10/9/92

NUMBER OF PAGES: 1

FAX (310) 203-3852

PHONE (310) 203-3959

A Professor at UCLA told me that you might be able to give me the answer to: What is the 40,000th digit of Pi?

We would like to use the answer in our show. Can you help?

Banned from book by 20th Century Fox

Peter Borwein's Observation

In 1996, Peter Borwein of SFU in Canada observed that the following well-known formula for $\log_e 2$

$$\log 2 = \sum_{n=1}^{\infty} \frac{1}{n2^n} = 0.693147180559945309942\ldots$$

leads to a simple scheme for computing binary digits at an arbitrary starting position (here {} denotes fractional part):

$$\begin{aligned} \left\{2^d \log 2\right\} &= \left\{\sum_{n=1}^{d} \frac{2^{d-n}}{n}\right\} + \sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n} \\ &= \left\{\sum_{n=1}^{d} \frac{2^{d-n} \bmod n}{n}\right\} + \sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n} \end{aligned}$$

Fast Exponentiation

The exponentiation (2^{d-n} mod n) in this formula can be evaluated very rapidly by means of the binary algorithm for exponentiation, performed modulo n:

Example:

$3^{17} = (((3^2)^2)^2)^2 \times 3 = 129140163$

In a similar way, we can evaluate:

$3^{17} \bmod 10 = ((((3^2 \bmod 10)^2 \bmod 10)^2 \bmod 10)^2 \bmod 10) \times 3 \bmod 10$

$3^2 \bmod 10 = 9$

$9^2 \bmod 10 = 1$

$1^2 \bmod 10 = 1$

$1^2 \bmod 10 = 1$

$1 \times 3 = 3$ Thus $3^{17} \bmod 10 = 3$.

Note: we never have to deal with integers larger than 81.

Is There an Arbitrary Digit Calculation Formula for Pi?

The same trick can be used for any mathematical constant given by a formula of the form

$$\alpha = \sum_{n=1}^{\infty} \frac{p(n)}{q(n)2^n}$$

where p and q are polynomials with integer coefficients, deg p < q, and q has no zeroes at positive integers. Any linear sum of such constants also has this property.

Is there a formula of this type for π? Until recently, none was known in mathematical literature.

The BBP Formula for Pi

In 1996, a PSLQ program discovered this formula for pi:

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

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.

So simple! Why wasn't it found hundreds of years ago?

Answer: Maybe it had to await the computer age – until recently no one would have thought to seek such a formula.

Proof of the BBP Formula

$$\int_0^{1/\sqrt{2}} \frac{x^{j-1}\,dx}{1-x^8} = \int_0^{1/\sqrt{2}} \sum_{k=0}^{\infty} x^{8k+j-1}\,dx = \frac{1}{2^{j/2}} \sum_{k=0}^{\infty} \frac{1}{16^k(8k+j)}$$

Thus

$$\begin{aligned}
\sum_{k=0}^{\infty} \frac{1}{16^k}\left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6}\right) \\
&= \int_0^{1/\sqrt{2}} \frac{(4\sqrt{2} - 8x^3 - 4\sqrt{2}x^4 - 8x^5)\,dx}{1-x^8} \\
&= \int_0^1 \frac{16(4 - 2y^3 - y^4 - y^5)\,dy}{16 - y^8} \\
&= \int_0^1 \frac{16(y-1)\,dy}{(y^2-2)(y^2-2y+2)} \\
&= \int_0^1 \frac{4y\,dy}{y^2-2)} - \int_0^1 \frac{(4y-8)\,dy}{y^2-2y+2} \\
&= \pi
\end{aligned}$$

Calculations Using the BBP Algorithm

Position	Hex Digits of Pi Starting at Position	
10^6	26C65E52CB4593	
10^7	17AF5863EFED8D	
10^8	ECB840E21926EC	
10^9	85895585A0428B	
10^{10}	921C73C6838FB2	
10^{11}	9C381872D27596	
1.25×10^{12}	07E45733CC790B	[1]
2.5×10^{14}	E6216B069CB6C1	[2]

[1] Babrice Bellard, France, 1999

[2] Colin Percival, Canada, 2000

Some Other Similar Identities

$$\pi\sqrt{3} = \frac{9}{32}\sum_{k=0}^{\infty}\frac{1}{64^k}\left(\frac{16}{6k+1}-\frac{8}{6k+2}-\frac{2}{6k+4}-\frac{1}{6k+5}\right)$$

$$\pi^2 = \frac{1}{8}\sum_{k=0}^{\infty}\frac{1}{64^k}\left(\frac{144}{(6k+1)^2}-\frac{216}{(6k+2)^2}-\frac{72}{(6k+3)^2}-\frac{54}{(6k+4)^2}+\frac{9}{(6k+5)^2}\right)$$

$$\pi^2 = \frac{2}{27}\sum_{k=0}^{\infty}\frac{1}{729^k}\left(\frac{243}{(12k+1)^2}-\frac{405}{(12k+2)^2}-\frac{81}{(12k+4)^2}-\frac{27}{(12k+5)^2}\right.$$
$$\left.-\frac{72}{(12k+6)^2}-\frac{9}{(12k+7)^2}-\frac{9}{(12k+8)^2}-\frac{5}{(12k+10)^2}+\frac{1}{(12k+11)^2}\right)$$

$$6\sqrt{3}\arctan\left(\frac{\sqrt{3}}{7}\right) = \sum_{k=0}^{\infty}\frac{1}{27^k}\left(\frac{3}{3k+1}+\frac{1}{3k+2}\right)$$

$$\frac{25}{2}\log\left(\frac{781}{256}\left(\frac{57-5\sqrt{5}}{57+5\sqrt{5}}\right)^{\sqrt{5}}\right) = \sum_{k=0}^{\infty}\frac{1}{5^{5k}}\left(\frac{5}{5k+2}+\frac{1}{5k+3}\right)$$

An Arctan Formula

$$
\begin{aligned}
\arctan\left(\frac{4}{5}\right) \quad = \quad & \frac{1}{2^{17}} \sum_{k=0}^{\infty} \frac{1}{2^{20k}} \left(\frac{524288}{40k+2} - \frac{393216}{40k+4} - \frac{491520}{40k+5} \right. \\
& + \frac{163840}{40k+8} + \frac{32768}{40k+10} - \frac{24576}{40k+12} + \frac{5120}{40k+15} \\
& + \frac{10240}{40k+16} + \frac{2048}{40k+18} + \frac{1024}{40k+20} + \frac{640}{40k+24} \\
& + \frac{480}{40k+25} + \frac{128}{40k+26} - \frac{96}{40k+28} + \frac{40}{40k+32} \\
& \left. + \frac{8}{40k+34} - \frac{5}{40k+35} - \frac{6}{40k+36} \right)
\end{aligned}
$$

Is There a Base-10 Formula for Pi?

Note that there is both a base-2 and a base-3 BBP-type formula for π^2. Base-2 and base-3 formulas are also known for a handful of other constants.

Question: Is there any base-n ($n \neq 2^b$) BBP-type formula for π?

Answer: No. This is ruled out in a new paper by Jon Borwein, David Borwein and Will Galway.

This does not rule out some completely different scheme for finding individual non-binary digits of π.

Normal Numbers

- A number is b-normal (or "normal base b") if every string of m digits in the base-b expansion appears with limiting frequency b^{-m}.
- Using measure theory, it is easy to show that almost all real numbers are b-normal, for any b.
- Widely believed to be b-normal, for any b:
  - π = 3.1415926535…
  - e = 2.7182818284…
  - Sqrt(2) = 1.4142135623…
  - Log(2) = 0.6931471805…
  - All irrational roots of polynomials with integer coefficients.

But to date there have been NO proofs for any of these. Proofs have been known only for contrived examples, such as C = 0.12345678910111213…

A Connection Between BBP Formulas and Normality

In 2001 Richard Crandall and I found a connection between BBP-type formulas and a class of iterative sequences. In particular, we found:

A mathematical constant given by a BBP-type formula is b-normal if and only if an associated iterative sequence is equidistributed in the unit interval.

This result relies crucially on the BBP formula for π and some other similar formulas, many of which were discovered using PSLQ computations.

A Class of Provably Normal Constants

Crandall and I have also shown (unconditionally) that an infinite class of mathematical constants is normal, including

$$\begin{aligned}\alpha_{2,3} &= \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k}} \\ &= 0.041883680831502985071252898624571682426096\ldots_{10} \\ &= \mathtt{0.0AB8E38F684BDA12F684BF35BA781948B0FCD6E9E0}\ldots_{16}\end{aligned}$$

$\alpha_{2,3}$ was proven 2-normal by Stoneham in 1971, but we have extended this to the case where (2,3) are any pair (p,q) of relatively prime integers. We also extended to uncountably infinite class, as follows [here r_k is the k-th bit of r in (0,1)]:

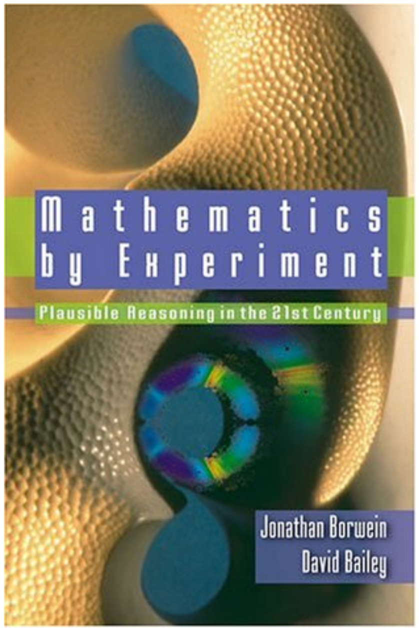
$$\alpha_{2,3}(r) = \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k + r_k}}$$

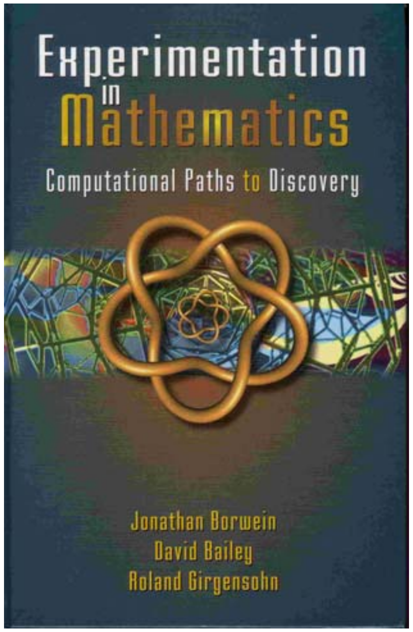
Two New Books on Experimental Mathematics

Vol. 1: Mathematics by Experiment: Plausible Reasoning in the 21st Century

Vol. 2: Experiments in Mathematics: Computational Paths to Discovery

Authors: Jonathan M Borwein and David H Bailey, with Roland Girgensohn for Vol. 2.





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