Experimentation in Mathematics: Plausible Reasoning in the 21st Century

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What Is Experimental Math?

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.

David Berlinski, 1997

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 Godel, 1951

The Experimental Methodology

- 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.

Experimental Math in Action

In 1988, Joseph Roy North observed that Gregory's series,

$$\pi = 4(1/3 - 1/5 + 1/7 - 1/9 + 1/11 - 1/13 + 1/15 \cdots)$$

when truncated to 5,000,000 terms, gives a value that differs strangely from the true value of pi:

```
3.14159245358979323846464338327950278419716939938730582097494182230781640...
3.14159265358979323846264338327950288419716939937510582097494459230781640...
        2             -2              10            -122             2770
```

Sloane's Encyclopedia of Integer Sequences, available at
http://www.research.att.com/~njas/sequences,
recognizes these integers as Euler numbers E_n. The above phenomenon is an artifact of the fact that 5,000,000 is one-half of a large power of ten.

The PSLQ Integer Relation Algorithm

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

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

- At the present time, the PSLQ algorithm of Helaman Ferguson is the most efficient algorithm for integer relation detection.
- PSLQ was named one of 10 "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

The PSLQ Algorithm

```
Initialize:  For j := 1 to n: for i := 1 to n: if i = j then set A_{i j} := 1 and B_{i j}
    := 1 else set A_{i j} := 0 and B_{i j} := 0; endfor; endfor.  For k := 1 to n: set
    s_k := sqrt {sum_{j=k}^n x_j^2}; endfor.  Set t := 1 / s_1.  For k := 1 to n: set y_k
    := t x_k; s_k := t s_k; endfor.
Initial H:  For j := 1 to n-1: for i := 1 to j-1: set H_{i j} := 0; endfor; set H_{j j}
    := s_{j+1}/s_j; for i := j+1 to n: set H_{i j} := - y_i y_j / (s_j s_{j+1}); endfor;
    endfor.
Reduce H:  For i := 2 to n: for j := i-1 to 1 step -1: set t := nint (H_{i j} / H_{j j});
    and y_j := y_j + t y_i; for k := 1 to j: set H_{i k} := H_{i k} - t H_{j k}; endfor;
    for k := 1 to n: set A_{i k} := A_{i k} - t A_{j k} and B_{k j} := B_{k j}
    + t B_{k i}; endfor; endfor; endfor.


Iterate:
Select m such that gamma^i |H_{i i}| is maximal when i = m.  Exchange the entries of y
    indexed m and m + 1, the corresponding rows of A and H, and the corresponding columns
    of B.
Remove corner on H diagonal:  If m <= n-2 then set t_0 := sqrt{H_{m m}^2 + H_{m,m+1}^2},
    t_1 := H_{m m} / t_0 and t_2 := H_{m,m+1} / t_0; for i := m to n: set t_3 := H_{i m},
    t_4 := H_{i, m+1}, H_{i m} := t_1 t_3 + t_2 t_4 and H_{i, m+1} := - t_2 t_3 + t_1
    t_4; endfor; endif.
Reduce H: For i := m+1 to n: for j := min(i-1, m+1) to 1 step -1: set t := nint (H_{i j}
    / H_{j j}) and y_j := y_j + t y_i; for k := 1 to j: set H_{i k} := H_{i k}
    - t H_{j k}; endfor; for k := 1 to n: set A_{i k} := A_{i k} - t A_{j k} and B_{k j}
    := B_{k j} + t B_{k i}; endfor; endfor; endfor.
Termination test:  If some y_i < epsilon, then a relation has been detected and is given
    in the corresponding column of B.
```

LBNL's Arbitrary Precision Computation (ARPREC) Package

- Written entirely in C++.
- C++ and F-90 translation modules permit this software to be used in programs with only minor changes to ordinary code.
- Double-double (32 digits), quad-double, (64 digits) and arbitrary precision (>64 digits) versions are available.
- Special routines for extra-high precision (>1000 digits).
- Includes common math functions: sqrt, cos, exp, log, etc.
- Includes PSLQ, root finding and numerical integration programs.

Authors: Brandon Thompson (UCB), Sherry Li (LBNL) Yozo Hida (UCB) and DHB.

An "Experimental Mathematician's Toolkit" (an interactive tool performing the above) is also available.

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

Identifying Algebraic Numbers Using PSLQ

Problem: Is a given real number α algebraic of degree *n* or less? I.e., is α the root of an algebraic equation with integer coefficients of degree *n* or less?

Solution: Compute the set of numbers

$$(1, \alpha, \alpha^2, \ldots, \alpha^n)$$

to high precision, and then apply the PSLQ algorithm.

Example (using Mathematician's Toolkit):

```
alpha = 3^0.25 – 2^0.25
pslq[table[alpha^k], {k, 0, 16}]
```

finds the following degree-16 polynomial:

$$0 = 1 - 3860t^4 - 666t^8 - 20t^{12} + t^{16}$$

Bifurcation Points in Chaos Theory

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

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

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

PSLQ can determine that B_3 satisfies

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

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

These results have subsequently been proven formally.

Fascination With Pi

Newton (1670):

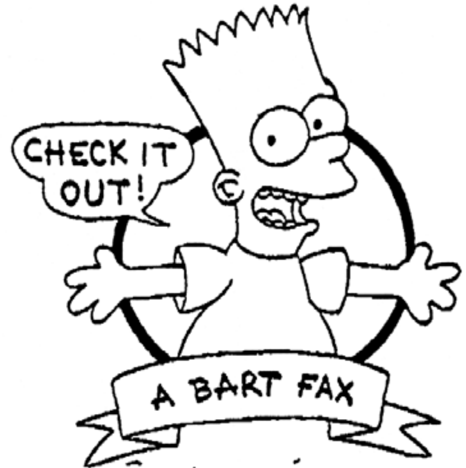
- "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."

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



TO: DAVID BAILEY

FROM: JACQUELINE ATKINS

DATE: 10/9/92

NUMBER OF PAGES: 1

FAX (310) 203-3852

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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?

Peter Borwein's Observation

In 1996, Peter Borwein (Simon Fraser Univ., Canada) observed that a well-known formula leads to a simple scheme for computing arbitrary binary digits of log 2.

(In the following, {} denotes fractional part):

$$\log 2 = \sum_{n=1}^{\infty} \frac{1}{n 2^n} = 0.69314718055994530...$$

$$\left\{2^d \log 2\right\} = \left\{\sum_{n=1}^{d} \frac{2^{d-n}}{n}\right\} + \left\{\sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n}\right\}$$

$$= \left\{\sum_{n=1}^{d} \frac{2^{d-n} \bmod n}{n}\right\} + \left\{\sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n}\right\}$$

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 (or any constant given by a sum of such formulas).

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

The BBP Formula for Pi

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

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

This formula permits one to directly calculate the *n*-th binary or hexadecimal (base 16) digit of pi, without needing to calculate any of the first *n*-1 digits.

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

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 we can write

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

$$= \int_0^{1/\sqrt{2}} \frac{(4\sqrt{2} - 8x^3 - 4\sqrt{2}x^4 - 8k^5)dx}{1-x^8}$$

$$= \int_0^1 \frac{16(4-2y^3-y^4-y^5)dy}{16-y^8}$$

$$= \int_0^1 \frac{16(y-1)dy}{(y^2-2)(y^2-2y+2)}$$

$$= \pi$$

Algorithm for Computing the n-th Hexadecimal Digit of Pi

Let S_1 be the first of the four sums in the formula for π. Then the hex expansion of S_1 beginning at position $n+1$ is:

$$\{16^n S_1\} = \left\{\sum_{k=0}^{\infty} \frac{16^{n-k}}{8k+1}\right\} = \left\{\sum_{k=0}^{n} \frac{16^{n-k}}{8k+1}\right\} + \left\{\sum_{k=n+1}^{\infty} \frac{16^{n-k}}{8k+1}\right\}$$

$$= \left\{\sum_{k=0}^{n} \frac{16^{n-k} \bmod 8k+1}{8k+1}\right\} + \left\{\sum_{k=n+1}^{\infty} \frac{16^{n-k}}{8k+1}\right\}$$

where $\{\}$ denotes fractional part. The numerator of the first summation can be evaluated very rapidly by means of the binary algorithm for exponentiation, where each multiplication is followed by reduction modulo $8k+1$. Only a few terms of the second summation need be evaluated, since it quickly converges. This computation is repeated for S_1, S_2, S_3, S_4.

The entire algorithm may be performed in ordinary 64-bit or 128-bit floating point arithmetic.

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 New Math Identities Found Using PSLQ

$$\log 3 = \sum_{k=0}^{\infty} \frac{1}{4^k (2k+1)}$$

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

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

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

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

An Arctan Formula

$$\tan^{-1}\left(\frac{1}{6}\right)=\frac{1}{2^{35}}\sum_{k=0}^{\infty}\frac{1}{2^{36k}}\left(\frac{2^{33}}{24k+1}-\frac{2^{32}}{24k+2}-\frac{2^{31}}{24k+3}-\frac{2^{27}}{24k+5}-\frac{2^{27}}{24k+6}\right)$$

$$+\frac{1}{2^{35}}\sum_{k=0}^{\infty}\frac{1}{2^{36k}}\left(-\frac{2^{24}}{24k+7}-\frac{2^{22}}{24k+9}-\frac{2^{20}}{24k+10}+\frac{2^{18}}{24k+11}-\frac{2^{15}}{24k+13}\right)$$

$$+\frac{1}{2^{35}}\sum_{k=0}^{\infty}\frac{1}{2^{36k}}\left(+\frac{2^{14}}{24k+14}+\frac{2^{13}}{24k+15}+\frac{2^{9}}{24k+17}+\frac{2^{9}}{24k+18}+\frac{2^{6}}{24k+19}\right)$$

$$+\frac{1}{2^{35}}\sum_{k=0}^{\infty}\frac{1}{2^{36k}}\left(+\frac{2^{4}}{24k+21}+\frac{2^{2}}{24k+22}-\frac{1}{24k+23}\right)$$

A Numerical Integration Solution

Using a high-precision numerical integration program, together with PSLQ, we found that if

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

then

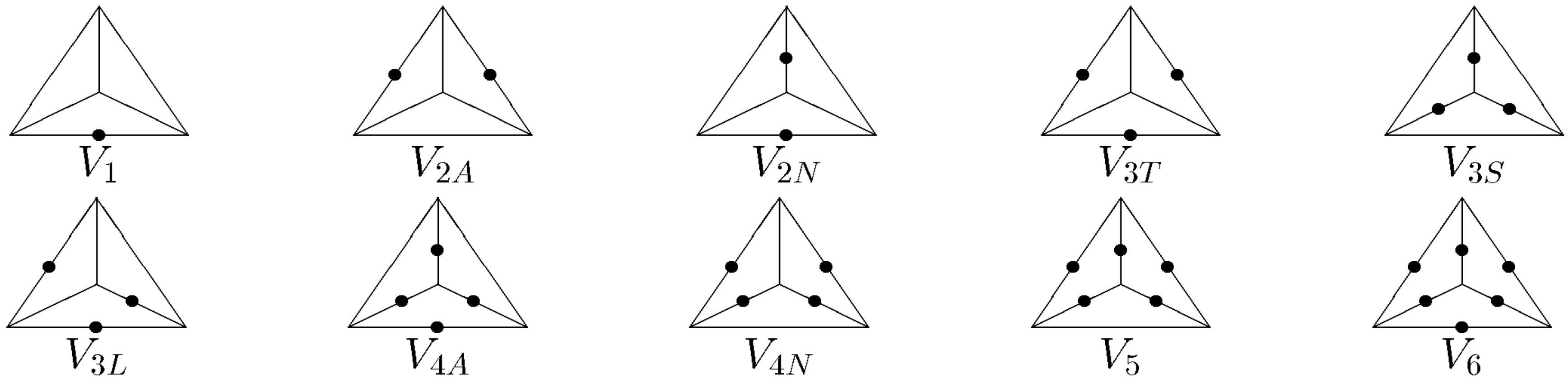
$$C(0) = (\pi \log 2)/8 + G/2$$

$$C(1) = \pi/4 - \pi\sqrt{2}/2 + 3\sqrt{2}\arctan(\sqrt{2})/2$$

$$C(\sqrt{2}) = 5\pi^2/96$$

where *G* is Catalan's constant. General formulas have now been established.

Evaluation of Ten Constants from Quantum Field Theory



$$V_1 = 6\zeta(3) + 3\zeta(4)$$

$$V_{2A} = 6\zeta(3) - 5\zeta(4)$$

$$V_{2N} = 6\zeta(3) - 13\zeta(4)/2 - 8U$$

$$V_{3T} = 6\zeta(3) - 9\zeta(4)$$

$$V_{3S} = 6\zeta(3) - 11\zeta(4)/2 - 4C^2$$

$$V_{3L} = 6\zeta(3) - 15\zeta(4) - 6C^2$$

$$V_{4A} = 6\zeta(3) - 77\zeta(4)/12 - 6C^2$$

$$V_{4N} = 6\zeta(3) - 14\zeta(4) - 16U$$

$$V_5 = 6\zeta(3) - 469\zeta(4)/27 + 8\zeta C^2/3 - 16V$$

$$V_6 = 6\zeta(3) - 13\zeta(4) - 8U - 4C^2$$

where

$$U = \sum_{j>k>0} (-1)^{j+k} / (j^3 k)$$

$$C = \sum_{k>0} \sin(\pi k/3)/k^2$$

$$V = \sum_{j>k>0} (-1)^j \cos(2\pi k/3)/(j^3 k)$$

PSLQ and Sculpture

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

$V = 2.0298832128193072500 42...$

Recently David Broadhurst found, using a PSLQ program, that V is given by a BBP-type formula:

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

Thus Ferguson's PSLQ algorithm solves Ferguson's sculpture!

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.

A Cautionary Example

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

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

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

$\ldots$

but

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

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

Cautionary Example II

$$\int_0^\infty \left[\cos(2x) \prod_{n=0}^{\infty} \cos(x/n) \right] dx =$$

0.392699081698724154807830422909937860524645434187231...

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

0.392699081698724154807830422909937860524646174921888...

These two constants agree to 42 digits, but are NOT equal.

Normal Numbers

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

But to date there have been NO proofs for any of these.

Proofs are only known for a handful of contrived examples, such as 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 normal base *b* if and only if an associated iterative sequence is equidistributed in the unit interval.

This result relies crucially on the BBP formula for pi and some other similar formulas discovered using PSLQ computations.

Example: Log_e 2

Consider the sequence (x_n) given by $x_0 = 0$, and

$$x_n = \{2x_{n-1} + 1/n\}$$

where {} denotes fractional part as before. Successive values of (x_n) appear to dance about randomly in the interval (0,1):

0.0000, 0.5000, 0.3333, 0.9167, 0.0333, 0.2333, 0.6095, 0.3440, 0.7992, 0.6984, 0.4877, 0.0588, 0.1945, 0.4605, 0.9876, 0.0378, 0.1344, 0.3243, 0.7012, 0.4524, 0.9524, 0.9502, 0.9439, 0.9295, ...

If it can be proven that (x_n) is equidistributed in the unit interval, then this would suffice to prove that log 2 is normal base 2.

The Iterative Sequence for Pi

The iterative sequence associated π with is $x_0 = 0$,

$$x_n = \left\{ 16x_{n-1} + \frac{120n^2 - 89n + 16}{512n^4 - 1024n^3 + 712n^2 - 206n + 21} \right\}$$

If it can be proven that the sequence (x_n) is equidistributed in the unit interval, then this would suffice to prove that π is normal base 16, and hence base 2 also.

Curious Fact:

Define the sequence (y_n) by $y_n = \{16x_n\}$. Then (y_n) appears to perfectly generate the hexadecimal expansion of π. We have verified this by computer to over 1,000,000 digits.

A Class of Provably Normal Constants

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

$$\alpha_{2,3} = \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k}}$$

= 0.041883680831502985071252... (decimal)

= 0.0AB8E38F684BDA12F684... (hexadecimal)

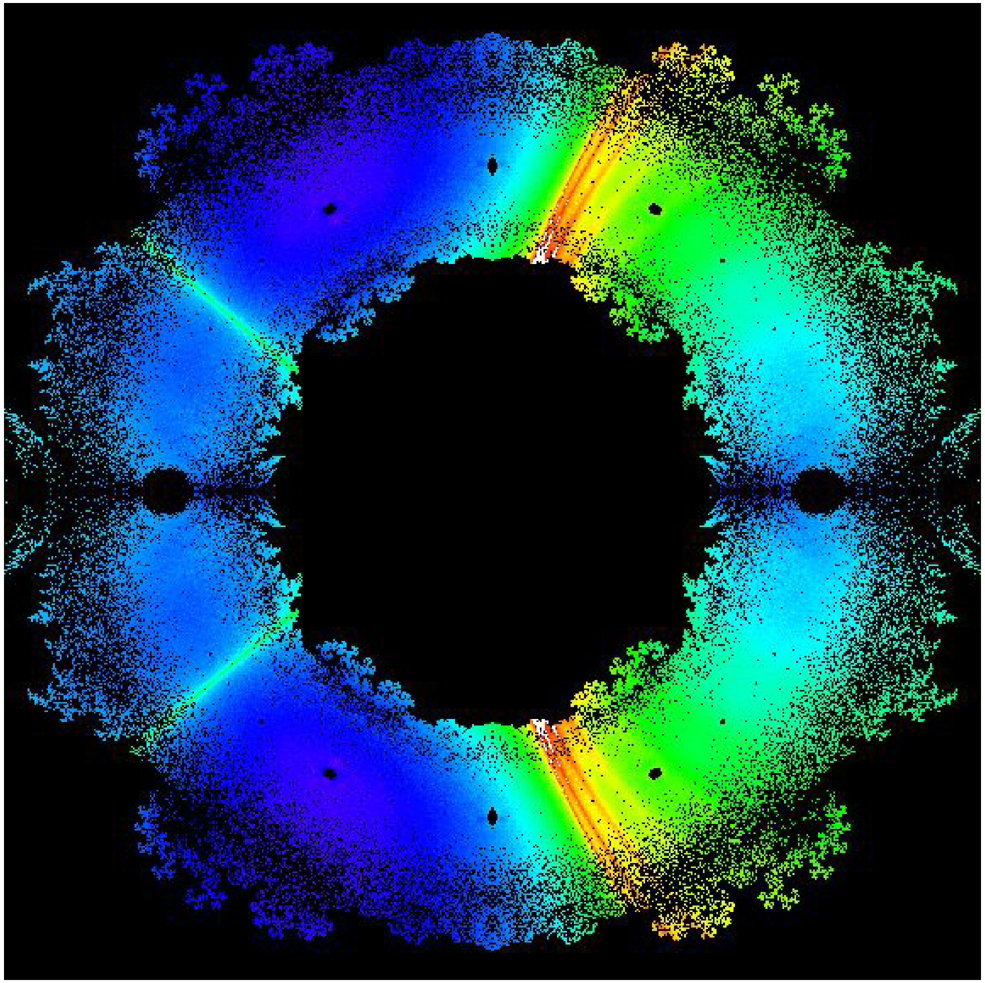
is normal. In particular, $\alpha_{2,3}$ is normal base 2.

Note: $\alpha_{2,3}$ was proven normal base 2 by Stoneham in 1973, but our results cover a much larger class.

An Unsolved Question of Experimental Mathematics

This is a plot of the complex roots of all polynomials up to degree 18 with coefficients in the set {-1, 0, 1}.

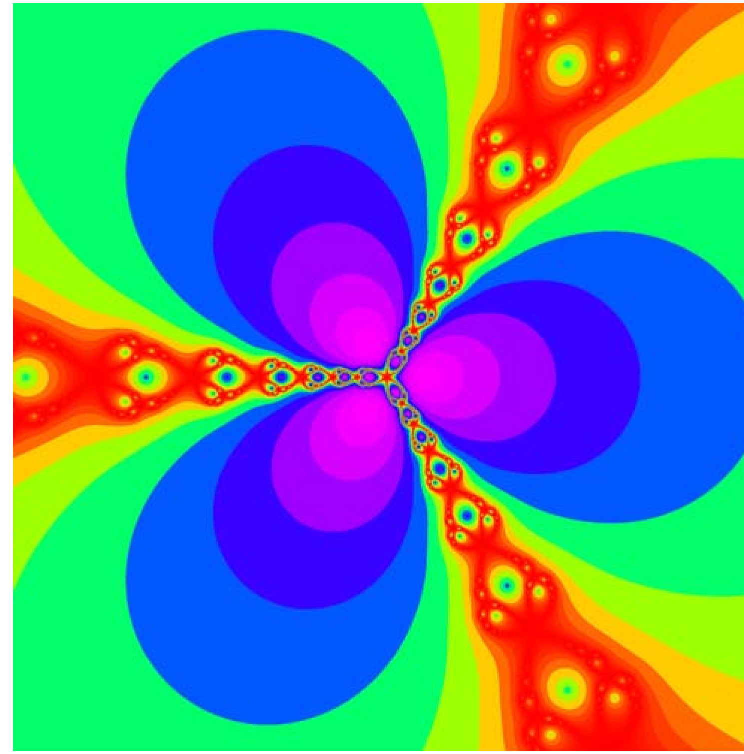
The bands, clearly visible in this plot, are unexplained.



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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A "Reader's Digest" condensed version is available FREE at **http://www.expmath.info**