Lattice sums arising from the Poisson equation

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Experimental mathematics:
Discovering new mathematical results by computer

Methodology:

1. Compute various mathematical entities (limits, infinite series sums, definite integrals, etc.) to high precision, typically 100–10,000 digits.
2. Use algorithms such as PSLQ to recognize these numerical values in terms of well-known mathematical constants.
3. When results are found experimentally, seek formal mathematical proofs of the discovered relations.

Many results have recently been found using this methodology, both in pure mathematics and in mathematical physics.

“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
The PSLQ integer relation algorithm

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

\[
a_1x_1 + a_2x_2 + \cdots + a_nx_n = 0
\]

(to within the “epsilon” of the arithmetic being used), or else finds bounds within which no relation can exist.

The “PSLQ” algorithm of mathematician-sculptor Helaman Ferguson is the most widely used integer relation algorithm.

Integer relation detection requires very high precision (at least \(n \times d\) digits, where \(d\) is the size in digits of the largest \(a_k\)), both in the input data and in the operation of the algorithm.

Efficient variants of PSLQ

- 2-level PSLQ performs almost all iterations with only double precision, updating full-precision arrays as needed. It is more than 100 times faster than the original PSLQ.
- 3-level PSLQ employs three levels of precision: double precision, intermediate precision (100-250 digits), and full precision (typically several thousand digits).
- Multipair PSLQ dramatically reduces the number of iterations required. It was designed for parallel systems, but runs faster even on 1 CPU.
- 2-level and 3-level variants are also available for multipair PSLQ. We now use 2-level multipair PSLQ for most work.

All of these are available on DHB’s high precision software website, together with the ARPREC arbitrary precision software:
http://www-legacy.lbl.gov/~dhbailey/mpdist
Operation of PSLQ

- PSLQ constructs a sequence of integer-valued matrices $B_n$ that reduce the vector $y = x \cdot B_n$, until either the relation is found (as one of the columns of matrix $B_n$), or else precision is exhausted.

- A relation is detected when the size of smallest entry of the $y$ vector suddenly drops to roughly “epsilon” (i.e. $10^{-p}$, where $p$ is the number of digits of precision).

- The size of this drop can be viewed as a “confidence level” that the relation is not a numerical artifact: a drop of 20+ orders of magnitude almost always indicates a real relation.
Decrease of $\log_{10}(\min |y_i|)$ in multipair PSLQ run
Computing arbitrary digits of log 2

In 1996, Peter Borwein of Simon Fraser University in Canada observed that the following well-known formula

$$\log 2 = \sum_{k=1}^{\infty} \frac{1}{k2^k} = 0.693147180559945\ldots$$

leads to a simple scheme for computing binary digits of log 2 at an arbitrary starting position (here \{\cdot\} denotes fractional part):

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

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

Is there a similar formula for \(\pi\)?
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:

\[3^{17} = (((3^2)^2)^2 \cdot 3 = 129140163\]

To obtain the result modulo an integer \(n\), just reduce each product modulo \(n\) before continuing.
The first major PSLQ discovery: The BBP formula for $\pi$

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

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

This formula permits one to compute binary (or hexadecimal) digits of $\pi$ beginning at an arbitrary starting position, using a very simple scheme that requires only standard 64-bit or 128-bit arithmetic.

In 2004, Borwein, Galway and Borwein proved that no base-$n$ formulas of this type exist for $\pi$, except when $n = 2^m$.

BBP-type formulas (discovered with PSLQ) are now known for numerous other mathematical constants.


Some other BBP-type formulas found using PSLQ programs

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

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

\[
\zeta(3) = \frac{1}{1792} \sum_{k=0}^{\infty} \frac{1}{2^{12k}} \left( \frac{6144}{(24k + 1)^3} - \frac{43008}{(24k + 2)^3} + \frac{24576}{(24k + 3)^3} + \frac{30720}{(24k + 4)^3} - \frac{1536}{(24k + 5)^3}
+ \frac{3072}{(24k + 6)^3} + \frac{768}{(24k + 7)^3} - \frac{3072}{(24k + 9)^3} - \frac{2688}{(24k + 10)^3} - \frac{192}{(24k + 11)^3} - \frac{1536}{(24k + 12)^3}
- \frac{96}{(24k + 13)^3} - \frac{672}{(24k + 14)^3} - \frac{384}{(24k + 15)^3} + \frac{24}{(24k + 17)^3} + \frac{48}{(24k + 18)^3}
- \frac{12}{(24k + 19)^3} + \frac{120}{(24k + 20)^3} + \frac{48}{(24k + 21)^3} - \frac{42}{(24k + 22)^3} + \frac{3}{(24k + 23)^3} \right)
\]

BBP-type formulas and normality

A constant is said to be 2-normal if every $m$-long string of binary digits appears, in the limit, with frequency $1/2^m$.

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

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

Then $\log 2$ is 2-normal if and only if the sequence $(x_n)$ is equidistributed in the unit interval.

Similarly consider the sequence defined by $x_0 = 0$ and

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

Then $\pi$ is 16-normal (and hence 2-normal) if and only if the sequence $(x_n)$ is equidistributed in the unit interval.

A class of provably normal constants

Consider Stoneham’s constant:

\[ \alpha_{2,3} = \sum_{k=0}^{\infty} \frac{1}{3^k 2^{3^k}} \]

\[ = 0.541883680831502985071252898\ldots_{10} \]

\[ = 0.8\text{ab8e38f684bda12f684bf35ba7}\ldots_{16} \]

Stoneham proved in 1971 that this constant is 2-normal. Crandall and I extended this to the uncountable class

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

where \( r_k \) is the \( k \)-th bit of a real number \( r \in (0, 1) \).

Misiurewicz and DHB recently proved the Stoneham result with a simpler argument, based on a lemma proven using ergodic theory.

High-precision tanh-sinh numerical integration

Given $f(x)$ defined on $(-1, 1)$, define $g(t) = \tanh(\pi/2 \sinh t)$. Then setting $x = g(t)$ yields

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

where $x_j = g(h_j)$ and $w_j = g'(h_j)$. Since $g'(t)$ goes to zero very rapidly for large $t$, the product $f(g(t))g'(t)$ typically is a nice bell-shaped function, so that the simple summation above converges very rapidly. Reducing $h$ by half typically doubles the number of correct digits.

We have found that tanh-sinh is the best general-purpose integration scheme for functions with vertical derivatives or singularities at endpoints, or for any function at very high precision ($> 1000$ digits). Otherwise we use Gaussian quadrature.

Ising integrals from mathematical physics

We recently applied our methods to study three classes of integrals. The $D_n$ integrals arise in the Ising theory of mathematical physics, while $C_n$ have connections to quantum field theory:

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

$$D_n := \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \prod_{i<j} \left(\frac{u_i-u_j}{u_i+u_j}\right)^2 \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

$$E_n = 2 \int_0^1 \cdots \int_0^1 \left(\prod_{1\leq j<k\leq n} \left(\frac{u_k-u_j}{u_k+u_j}\right)\right)^2 dt_2 \, dt_3 \cdots \, dt_n$$

where in the last line $u_k = t_1 t_2 \cdots t_k$.

Limiting value of $C_n$: What is this number?

Key observation: The $C_n$ integrals can be converted to one-dimensional integrals involving the modified Bessel function $K_0(t)$:

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

High-precision numerical values, computed using this formula and tanh-sinh quadrature, approach a limit. For example:

$$C_{1024} = 0.6304735033743867961220401927108789043545870787\ldots$$

What is this number? We copied the first 50 digits into the online Inverse Symbolic Calculator (ISC) at http://carma-lx1.newcastle.edu.au:8087. The result was:

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

where $\gamma$ denotes Euler’s constant. This is now proven.
Other Ising integral evaluations found using a multipair PSLQ program

\[ D_2 = 1/3 \]
\[ D_3 = 8 + 4\pi^2/3 - 27 L_{-3}(2) \]
\[ D_4 = 4\pi^2/9 - 1/6 - 7\zeta(3)/2 \]
\[ E_2 = 6 - 8 \log 2 \]
\[ E_3 = 10 - 2\pi^2 - 8 \log 2 + 32 \log^2 2 \]
\[ E_4 = 22 - 82\zeta(3) - 24 \log 2 + 176 \log^2 2 - 256(\log^3 2)/3 \]
\[ +16\pi^2 \log 2 - 22\pi^2/3 \]
\[ E_5 = 42 - 1984 \text{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3) \log 2 \]
\[ +40\pi^2 \log^2 2 - 62\pi^2/3 + 40(\pi^2 \log 2)/3 + 88 \log^4 2 \]
\[ +464 \log^2 2 - 40 \log 2 \]

where \( \zeta \) is the Riemann zeta function and \( \text{Li}_n(x) \) is the polylog function. \( D_2, D_3 \) and \( D_4 \) were originally provided to us by Craig Tracy, who hoped that our tools could help identify \( D_5 \).
The Ising integral $E_5$

We were able to reduce $E_5$, which is a 5-D integral, to an extremely complicated 3-D integral (see right).

We computed this integral to 250-digit precision, with a highly parallel, high-precision 3-D quadrature program. Then we used a PSLQ program to discover the evaluation given on the previous page.

We also computed $D_5$ to 500 digits, but were unable to identify it. The digits are available if anyone wishes to further explore.
Poisson potential functions and associated lattice sums

The Poisson equation arises in numerous applied mathematical contexts, including engineering applications, the analysis of crystal structures, and even the sharpening of photographic images.

The following lattice sums arise as values of basis functions in the Poisson solutions:

\[
\phi_n(r_1, \ldots, r_n) = \frac{1}{\pi^2} \sum_{m_1, \ldots, m_n \text{ odd}} e^{i\pi (m_1 r_1 + \cdots + m_n r_n)} \frac{1}{m_1^2 + \cdots + m_n^2}.
\]


Computing high-precision numerical values of such sums was facilitated by deriving formulas such as

\[
\phi_2(x, y) = \frac{1}{4\pi} \log \frac{\cosh(\pi x) + \cos(\pi y)}{\cosh(\pi x) - \cos(\pi y)} - \frac{2}{\pi} \sum_{m \in \mathbb{Z}^+} \frac{\cosh(\pi mx) \cos(\pi my)}{m(1 + e^{\pi m})},
\]

which is valid for \( x, y \in [-1, 1] \).
After extensive computational experimentation, we numerically discovered the remarkable fact that in the simplest two-dimensional case, for rational \((x, y)\), the Poisson potential function satisfies

\[
\phi_2(x, y) = \frac{1}{\pi^2} \sum_{m,n \text{ odd}} \frac{\cos(m\pi x) \cos(n\pi y)}{m^2 + n^2} = \frac{1}{\pi} \log \alpha
\]

where \(\alpha\) is algebraic, i.e., the root of an integer polynomial

\[
0 = a_0 + a_1 \alpha + a_2 \alpha^2 + \cdots + a_n \alpha^n
\]

This numerical observation has now been proven rigorously.
1. Let $\alpha = 8 \exp(\pi \phi_2(x, y))$. We found that the resulting polynomials were of lower degree, and thus much easier to numerically find, by inserting “8”.

2. Compute, to very high precision (typically thousands of digits) the $(n + 1)$-long vector $X = (1, \alpha, \alpha^2, \cdots, \alpha^n)$.

3. Feed the vector $X$ to a multipair PSLQ program (with similarly high precision). The multipair PSLQ returns the vector of integer coefficients $(a_0, a_1, a_2, \cdots, a_n)$ as output.
Samples of minimal polynomials found by PSLQ

\[ k \quad \text{Minimal polynomial for } \exp(8\pi \phi_2(1/k, 1/k)) \]

5 \[ 1 + 52\alpha - 26\alpha^2 - 12\alpha^3 + \alpha^4 \]
6 \[ 1 - 28\alpha + 6\alpha^2 - 28\alpha^3 + \alpha^4 \]
7 \[ -1 - 196\alpha + 1302\alpha^2 - 14756\alpha^3 + 15673\alpha^4 + 42168\alpha^5 - 111916\alpha^6 + 82264\alpha^7 \]
\[ -35231\alpha^8 + 19852\alpha^9 - 2954\alpha^{10} - 308\alpha^{11} + 7\alpha^{12} \]
8 \[ 1 - 88\alpha + 92\alpha^2 - 872\alpha^3 + 1990\alpha^4 - 872\alpha^5 + 92\alpha^6 - 88\alpha^7 + \alpha^8 \]
9 \[ -1 - 534\alpha + 10923\alpha^2 - 342864\alpha^3 + 2304684\alpha^4 - 7820712\alpha^5 + 13729068\alpha^6 \]
\[ -22321584\alpha^7 + 39775986\alpha^8 - 44431044\alpha^9 + 19899882\alpha^{10} + 3546576\alpha^{11} \]
\[ -8458020\alpha^{12} + 4009176\alpha^{13} - 273348\alpha^{14} + 121392\alpha^{15} \]
\[ -11385\alpha^{16} - 342\alpha^{17} + 3\alpha^{18} \]
10 \[ 1 - 216\alpha + 860\alpha^2 - 744\alpha^3 + 454\alpha^4 - 744\alpha^5 + 860\alpha^6 - 216\alpha^7 + \alpha^8 \]

The minimal polynomial for \( \exp(8\pi \phi_2(1/32, 1/32)) \) has degree 128, with individual coefficients ranging from 1 to over \( 10^{56} \). This PSLQ computation required 10,000-digit precision. See next page.

Other polynomials required up to 50,000-digit precision.
Degree-128 minimal polynomial for $\exp(8\pi\phi_2(1/32, 1/32))$
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Table: Minimal polynomials satisfied by $\exp(8\pi \phi_2(1/d, 1/d))$. 
Curious number-theoretic formula for the degree $m(d)$

As Jason Kimberley has observed empirically the degree of the polynomial $m(d)$ in the previous table appears to be given for odd primes by

$$m(4k + 1) = (2k) \cdot (2k)$$
$$m(4k + 3) = (2k + 2) \cdot (2k + 1)$$

If we set $m(2) = 1/2$, for notational convenience, then it seems that for any prime factorization of an integer greater than 2:

$$m\left(\prod_{i=1}^{k} p_i^{e_i}\right) \overset{?}{=} 4^{k-1} \prod_{i=1}^{k} p_i^{2(e_i-1)} m(p_i)$$

This sequence now appears as [http://oeis.org/A218147](http://oeis.org/A218147) in the *Online Encyclopedia of Integer Sequences*. 
This talk is available at http://www.davidhbailey.com/dhbtalks/dhb-poisson-sums.pdf.

The Poisson lattice work is written up in these papers:
