PSLQ: An algorithm to discover mathematical identities

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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*

Free software for high-precision computation

1. ARPREC. Arbitrary precision, with numerous algebraic and transcendental functions. High-level interfaces for C++ and Fortran-90. http://crd.lbl.gov/~dhbailey/mpdist.
2. GMP. Produced by a volunteer effort and distributed under the GNU license. http://gmplib.org.
3. MPFR. C library for multiple-precision floating-point computations with exact rounding, based on GMP. http://www.mpfr.org.
4. MPFR++. High-level C++ interface to MPFR. http://perso.ens-lyon.fr/nathalie.revol/software.html.
5. MPFUN90. Similar to ARPREC, but is written entirely in Fortran-90 and provides only a Fortran-90 interface. http://crd.lbl.gov/~dhbailey/mpdist.
6. QD. Performs "double-double" (31 digits) and "quad-double" (62 digits) arithmetic. High-level interfaces for C++ and Fortran-90. http://crd.lbl.gov/~dhbailey/mpdist.

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

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

(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.

1. H.R.P. Ferguson, D.H. Bailey and S. Arno, "Analysis of PSLQ, An Integer Relation Finding Algorithm," *Mathematics of Computation*, vol. 68, no. 225 (Jan 1999), pg. 351–369.
2. D.H. Bailey and D.J. Broadhurst, "Parallel Integer Relation Detection: Techniques and Applications," *Mathematics of Computation*, vol. 70, no. 236 (Oct 2000), pg. 1719–1736.

Efficient variants of PSLQ

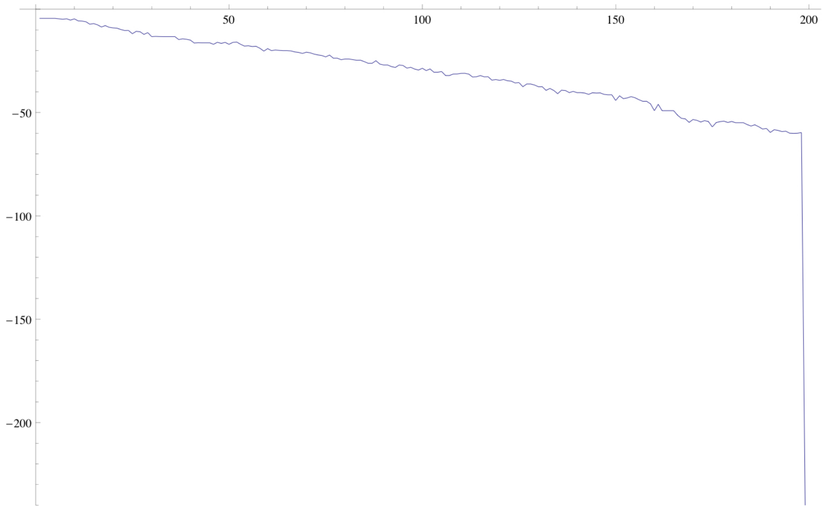
- 2-level PSLQ performs almost all iterations with only double precision, updating full-precision arrays as needed. It is more than 100 times faster than the original PSLQ.
- 3-level PSLQ employs three levels of precision: double precision, intermediate precision (100-250 digits), and full precision (typically several thousand digits).
- Multi-pair 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 multi-pair PSLQ.

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):

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

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:

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

In a similar way, we can evaluate

$$\begin{aligned}
3^{17} \bmod 10 &= ((((3^2 \bmod 10)^2 \bmod 10)^2 \bmod 10)^2 \bmod 10) \cdot 3 \bmod 10 \\
3^2 \bmod 10 &= 9 \\
9^2 \bmod 10 &= 1 \\
1^2 \bmod 10 &= 1 \\
1^2 \bmod 10 &= 1 \\
1 \cdot 3 &= 3
\end{aligned}$$

Thus $3^{17} \bmod 10 = 3$. Note that we never deal with integers > 81.

Is there a similar formula for π?

The same technique can be applied for any mathematical constant given by a formula of the form

$$\alpha = \sum_{k=0}^{\infty} \frac{p(k)}{q(k)2^k}$$

where $p(k)$ and $q(k)$ are polynomials with integer coefficients, $\deg(p) < \deg(q)$, and $q(k)$ has no zeroes at non-negative integers (so denominator is not zero). Any linear sum of such constants also has this property.

In 1996, no such formula of this type for π was known in the mathematical literature.

The first major PSLQ discovery: The BBP formula for π

In 1996, a PSLQ program discovered this new formula for π:

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

This formula permits one to compute binary (or hexadecimal) digits of π 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 π, except when $n = 2^m$.

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

1. D.H. Bailey, P.B. Borwein and S. Plouffe, "On the rapid computation of various polylogarithmic constants," *Mathematics of Computation*, vol. 66, no. 218 (Apr 1997), pg. 903–913.
2. J.M. Borwein, W.F. Galway and D. Borwein, "Finding and excluding b-ary Machin-type BBP formulae," *Canadian Journal of Mathematics*, vol. 56 (2004), pg. 1339–1342.

Some other BBP-type formulas found using PSLQ

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

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

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

D.H. Bailey, J.M. Borwein, A. Mattingly, and G. Wightwick, "The Computation of Previously Inaccessible Digits of π^2 and Catalan's Constant," *Notices of the AMS*, in press, 2013.

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 π is 16-normal (and hence 2-normal) if and only if the sequence (x_n) is equidistributed in the unit interval.

D.H. Bailey and R.E. Crandall, "On the random character of fundamental constant expansions," *Experimental Mathematics*, vol. 10, no. 2 (Jun 2001), pg. 175-190.

A class of provably normal constants

Consider Stoneham's constant:

$$\alpha_{2,3} = \sum_{k=0}^{\infty} \frac{1}{3^k 2^{3^k}}$$
$$= 0.541883680831502985071252898\ldots_{10}$$
$$= 0.8ab8e38f684bda12f684bf35ba7\ldots_{16}$$

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.

1. D.H. Bailey and R.E. Crandall, "Random generators and normal numbers," *Experimental Mathematics*, vol. 11, no. 4 (2002), pg. 527-546.
2. D.H. Bailey and M. Misiurewicz, "A strong hot spot theorem," *Proceedings of the American Mathematical Society*, vol. 134 (2006), no. 9, pg. 2495-2501.

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.

1. D.H. Bailey, X.S. Li and K. Jeyabalan, "A Comparison of Three High-Precision Quadrature Schemes," *Experimental Mathematics*, vol. 14 (2005), no. 3, pg. 317–329.
2. H. Takahasi and M. Mori, "Double Exponential Formulas for Numerical Integration," *Publications of RIMS*, Kyoto University, vol. 9 (1974), pg. 721-741.

Ising integrals from mathematical physics

We recently applied our methods to study three classes of integrals (one of which was referred to us by Craig Tracy of U.C. Davis) that arise in the Ising theory of mathematical physics:

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

$$D_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{\prod_{i<j}\left(\frac{u_i-u_j}{u_i+u_j}\right)^2}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{\mathrm{d}u_1}{u_1} \cdots \frac{\mathrm{d}u_n}{u_n}$$

$$E_n = 2\int_0^1 \cdots \int_0^1 \left(\prod_{1\le j<k\le n} \frac{u_k - u_j}{u_k + u_j}\right)^2 \mathrm{d}t_2\, dt_3 \cdots \mathrm{d}t_n$$

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

D.H. Bailey, J.M. Borwein and R.E. Crandall, "Integrals of the Ising class," *Journal of Physics A: Mathematical and General*, vol. 39 (2006), pg. 12271–12302.

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 $K_0(t)$:

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

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 γ denotes Euler's constant. This is now proven.

Other Ising integral evaluations found using PSLQ

$$
\begin{aligned}
D_2 &= 1/3 \\
D_3 &= 8 + 4\pi^2/3 - 27\,\mathrm{L}_{-3}(2) \\
D_4 &= 4\pi^2/9 - 1/6 - 7\zeta(3)/2 \\
E_2 &= 6 - 8\log 2 \\
E_3 &= 10 - 2\pi^2 - 8\log 2 + 32\log^2 2 \\
E_4 &= 22 - 82\zeta(3) - 24\log 2 + 176\log^2 2 - 256(\log^3 2)/3 \\
&\quad +16\pi^2\log 2 - 22\pi^2/3 \\
E_5 &\stackrel{?}{=} 42 - 1984\,\mathrm{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3)\log 2 \\
&\quad +40\pi^2\log^2 2 - 62\pi^2/3 + 40(\pi^2\log 2)/3 + 88\log^4 2 \\
&\quad +464\log^2 2 - 40\log 2
\end{aligned}
$$

where ζ is the Riemann zeta function and $Li_n(x)$ 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 E5, which is a 5-D integral, to an extremely complicated 3-D integral (see right).

We computed this integral to 250-digit precision, using 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.

$$
\begin{aligned}
E_5 \;=\; & \int_0^1 \int_0^1 \int_0^1 [2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 \\
& (-[4(x+1)(xy+1)\log(2)(y^5z^3x^7 - y^4z^2(4(y+1)z+3)x^6 - y^3z((y^2+1)z^2+4(y+ \\
& 1)z+5)x^5 + y^2(4y(y+1)z^3+3(y^2+1)z^2+4(y+1)z-1)x^4 + y(z(z^2+4z \\
& +5)y^2+4(z^2+1)y+5z+4)x^3 + ((-3z^2-4z+1)y^2-4zy+1)x^2 - (y(5z+4) \\
& +4)x-1)] / [(x-1)^3(xy-1)^3(xyz-1)^3] + [3(y-1)^2y^4(z-1)^2z^2(yz \\
& -1)^2x^6 + 2y^3z(3(z-1)^2z^3y^5 + z^2(5z^3+3z^2+3z+5)y^4 + (z-1)^2z \\
& (5z^2+16z+5)y^3 + (3z^5+3z^4-22z^3-22z^2+3z+3)y^2 + 3(-2z^4+z^3+2 \\
& z^2+z-2)y + 3z^3+5z^2+5z+3)x^5 + y^2(7(z-1)^2z^4y^6 - 2z^3(z^3+15z^2 \\
& +15z+1)y^5 + 2z^2(-21z^4+6z^3+14z^2+6z-21)y^4 - 2z(z^5-6z^4-27z^3 \\
& -27z^2-6z+1)y^3 + (7z^6-30z^5+28z^4+54z^3+28z^2-30z+7)y^2 - 2(7z^5 \\
& +15z^4-6z^3-6z^2+15z+7)y + 7z^4-2z^3-42z^2-2z+7)x^4 - 2y(z^3(z^3 \\
& -9z^2-9z+1)y^6 + z^2(7z^4-14z^3-18z^2-14z+7)y^5 + z(7z^5+14z^4+3 \\
& z^3+3z^2+14z+7)y^4 + (z^6-14z^5+3z^4+84z^3+3z^2-14z+1)y^3 - 3(3z^5 \\
& +6z^4-z^3-z^2+6z+3)y^2 - (9z^4+14z^3-14z^2+14z+9)y + z^3+7z^2+7z \\
& +1)x^3 + (z^2(11z^4+6z^3-66z^2+6z+11)y^6 + 2z(5z^5+13z^4-2z^3-2z^2 \\
& +13z+5)y^5 + (11z^6+26z^5+44z^4-66z^3+44z^2+26z+11)y^4 + (6z^5-4 \\
& z^4-66z^3-66z^2-4z+6)y^3 - 2(33z^4+2z^3-22z^2+2z+33)y^2 + (6z^3+26 \\
& z^2+26z+6)y + 11z^2+10z+11)x^2 - 2(z^2(5z^3+3z^2+3z+5)y^5 + z(22z^4 \\
& +5z^3-22z^2+5z+22)y^4 + (5z^5+5z^4-26z^3-26z^2+5z+5)y^3 + (3z^4- \\
& 22z^3-26z^2-22z+3)y^2 + (3z^3+5z^2+5z+3)y + 5z^2+22z+5)x + 15z^2+2z \\
& +2y(z-1)^2(z+1) + 2y^3(z-1)^2z(z+1) + y^4z^2(15z^2+2z+15) + y^2(15z^4 \\
& -2z^3-90z^2-2z+15)+15] / [(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2 \\
& (xyz-1)^2] - [4(x+1)(y+1)(yz+1)(-z^2y^4+4z(z+1)y^3+(z^2+1)y^2 \\
& -4(z+1)y+4x(y^2-1)(y^2z^2-1)+x^2(z^2y^4-4z(z+1)y^3-(z^2+1)y^2 \\
& +4(z+1)y+1)-1)\log(x+1)] / [(x-1)^3x(y-1)^3(yz-1)^3] - [4(y+1)(xy \\
& +1)(z+1)(x^2(z^2-4z-1)y^4+4x(x+1)(z^2-1)y^3-(x^2+1)(z^2-4z-1) \\
& y^2-4(x+1)(z^2-1)y+z^2-4z-1)\log(xy+1)] / [x(y-1)^3y(xy-1)^3(z- \\
& 1)^3] - [4(z+1)(yz+1)(x^3y^5z^7+x^2y^4(4x(y+1)+5)z^6-xy^3((y^2+ \\
& 1)x^2-4(y+1)x-3)z^5-y^2(4y(y+1)x^3+5(y^2+1)x^2+4(y+1)x+1)z^4+ \\
& y(y^2x^3-4y(y+1)x^2-3(y^2+1)x-4(y+1))z^3+(5x^2y^2+y^2+4x(y+1) \\
& y+1)z^2+((3x+4)y+4)z-1)\log(xyz+1)] / [xy(z-1)^3z(yz-1)^3(xyz-1)^3])] \\
& / [(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2] \, dx\,dy\,dz
\end{aligned}
$$

Recursions in Ising integrals

Consider the 2-parameter class of Ising integrals (which arises in quantum field theory for odd k):

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

After computing 1000-digit numerical values for all n up to 36 and all k up to 75, we discovered (using PSLQ) linear relations in the rows of this array. For example, when $n = 3$:

$$\begin{aligned}
0 &= C_{3,0} - 84 C_{3,2} + 216 C_{3,4} \\
0 &= 2 C_{3,1} - 69 C_{3,3} + 135 C_{3,5} \\
0 &= C_{3,2} - 24 C_{3,4} + 40 C_{3,6} \\
0 &= 32 C_{3,3} - 630 C_{3,5} + 945 C_{3,7} \\
0 &= 125 C_{3,4} - 2172 C_{3,6} + 3024 C_{3,8}
\end{aligned}$$

Similar recursions have been found (and proven) for all n.

1. D.H. Bailey, D. Borwein, J.M. Borwein and R.E. Crandall, "Hypergeometric Forms for Ising-Class Integrals," *Experimental Mathematics*, vol. 16 (2007), pg. 257–276.
2. J.M. Borwein and B. Salvy, "A Proof of a Recursion for Bessel Moments," *Experimental Mathematics*, vol. 17 (2008), pg. 223–230.

Box integrals

The following integrals appear in numerous applications:

$$B_n(s) := \int_0^1 \cdots \int_0^1 \left(r_1^2 + \cdots + r_n^2\right)^{s/2} \, \mathrm{d}R$$

$$\Delta_n(s) := \int_0^1 \cdots \int_0^1 \left((r_1 - q_1)^2 + \cdots + (r_n - q_n)^2\right)^{s/2} \, \mathrm{d}R\mathrm{d}Q$$

- $B_n(1)$ is average distance of a random point from the origin.
- $\Delta_n(1)$ is average distance between two random points.
- $B_n(-n+2)$ is average electrostatic potential in an n-cube whose origin has a unit charge.
- $\Delta_n(-n+2)$ is average electrostatic energy between two points in a uniform n-cube of charged "jellium."
- Recently integrals of this type have arisen in neuroscience, e.g. the average distance between synapses in a mouse brain.

D.H. Bailey, J.M. Borwein and R.E. Crandall, "Box integrals," *Journal of Computational and Applied Mathematics*, vol. 206 (2007), pg. 196–208.

Sample evaluations of box integrals

n	s	$B_n(s)$
any	even $s \geq 0$	rational, e.g., : $B_2(2) = 2/3$
1	$s \neq -1$	$\frac{1}{s+1}$
2	-4	$-\frac{1}{4} - \frac{\pi}{8}$
2	-3	$-\sqrt{2}$
2	-1	$2\log(1+\sqrt{2})$
2	1	$\frac{1}{3}\sqrt{2} + \frac{1}{3}\log(1+\sqrt{2})$
2	3	$\frac{7}{5}\sqrt{2} + \frac{3}{20}\log(1+\sqrt{2})$
2	$s \neq -2$	$\frac{2}{2+s}\ {}_2F_1\left(\frac{1}{2}, -\frac{s}{2}; \frac{3}{2}; -1\right)$
3	-5	$-\frac{1}{6}\sqrt{3} - \frac{1}{12}\pi$
3	-4	$-\frac{3}{2}\sqrt{2}\arctan\frac{1}{\sqrt{2}}$
3	-2	$-3G + \frac{3}{2}\pi\log(1+\sqrt{2}) + 3\ \mathrm{Ti}_2(3-2\sqrt{2})$
3	-1	$-\frac{1}{4}\pi + \frac{3}{2}\log\left(2+\sqrt{3}\right)$
3	1	$\frac{1}{4}\sqrt{3} - \frac{1}{24}\pi + \frac{1}{2}\log\left(2+\sqrt{3}\right)$
3	3	$\frac{2}{5}\sqrt{3} - \frac{1}{60}\pi - \frac{7}{20}\log\left(2+\sqrt{3}\right)$

Here F is hypergeometric function; G is Catalan; Ti is Lewin's inverse-tan function.

Elliptic integral functions

Research with "ramble" integrals led us to consider these integrals:

$$I(n_0, n_1, n_2, n_3, n_4) \quad := \quad \int_0^1 x^{n_0} K^{n_1}(x) K'^{n_2}(x) E^{n_3}(x) E'^{n_4}(x) \mathrm{d}x,$$

where K, K', E, E' are elliptic integral functions:

$$\begin{aligned} K(x) &:= \int_0^1 \frac{\mathrm{d}t}{\sqrt{(1-t^2)(1-x^2t^2)}} \\ K'(x) &:= K(\sqrt{1-x^2}) \\ E(x) &:= \int_0^1 \frac{\sqrt{1-x^2t^2}}{\sqrt{1-t^2}} \, \mathrm{d}t \\ E'(x) &:= E(\sqrt{1-x^2}) \end{aligned}$$

1. J. Wan, "Moments of products of elliptic integrals," *Advances in Applied Mathematics*, vol. 48 (2012), pg. 121–141, `http://carma.newcastle.edu.au/jamesw/mkint.pdf`.
2. D.H. Bailey and J.M. Borwein, "Hand-to-hand combat with thousand-digit integrals," *Journal of Computational Science*, vol. 3 (2012), pg. 77–86, `http://www.davidhbailey.com/dhbpapers/combat.pdf`.

Relations found among the I integrals

Thousands of relations have been found among the I integrals. For example, among the class with $n_0 \leq D_1 = 4$ and $n_1 + n_2 + n_3 + n_4 = D_2 = 3$ (a set of 100 integrals), we found that all can be expressed in terms of an integer linear combination of 8 simple integrals. Some examples:

$$\begin{aligned}
81 \int_0^1 x^3 K^2(x) E(x) \mathrm{d}x &\stackrel{?}{=} -6 \int_0^1 K^3(x) \mathrm{d}x - 24 \int_0^1 x^2 K^3(x) \mathrm{d}x \\
&+51 \int_0^1 x^3 K^3(x) \mathrm{d}x + 32 \int_0^1 x^4 K^3(x) \mathrm{d}x \\
-243 \int_0^1 x^3 K(x) E(x) K'(x) \mathrm{d}x &\stackrel{?}{=} -59 \int_0^1 K^3(x) \mathrm{d}x + 468 \int_0^1 x^2 K^3(x) \mathrm{d}x \\
&+156 \int_0^1 x^3 K^3(x) \mathrm{d}x - 624 \int_0^1 x^4 K^3(x) \mathrm{d}x - 135 \int_0^1 x K(x) E(x) K'(x) \mathrm{d}x \\
-20736 \int_0^1 x^4 E^2(x) K'(x) \mathrm{d}x &\stackrel{?}{=} 3901 \int_0^1 K^3(x) \mathrm{d}x - 3852 \int_0^1 x^2 K^3(x) \mathrm{d}x \\
&-1284 \int_0^1 x^3 K^3(x) \mathrm{d}x + 5136 \int x^4 K^3(x) \mathrm{d}x - 2592 \int_0^1 x^2 K^2(x) K'(x) \mathrm{d}x \\
&-972 \int_0^1 K(x) E(x) K'(x) \mathrm{d}x - 8316 \int_0^1 x K(x) E(x) K'(x) \mathrm{d}x.
\end{aligned}$$

Algebraic numbers in Poisson potential functions associated with lattice sums

Lattice sums arising from the Poisson equation have been studied widely in mathematical physics and also in image processing. We numerically discovered, and then proved, that for rational (x, y), the two-dimensional 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 α is *algebraic*, i.e., the root of an integer polynomial

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

The minimal polynomials for these α were found by PSLQ calculations, with the $(n+1)$-long vector $(1, \alpha, \alpha^2, \cdots, \alpha^n)$ as input, where $\alpha = \exp(\pi\phi_2(x,y))$. PSLQ returns the vector of integer coefficients $(a_0, a_1, a_2, \cdots, a_n)$ as output.

1. D.H. Bailey, J.M. Borwein, R.E. Crandall and J. Zucker, "Lattice sums arising from the Poisson equation," *Journal of Physics A: Mathematical and Theoretical*, vol. 46 (2013), pg. 115201, http://www.davidhbailey.com/dhbpapers/PoissonLattice.pdf.
2. D.H. Bailey and J.M. Borwein, "Compressed lattice sums arising from the Poisson equation: Dedicated to Professor Hari Sirvastava," manuscript, http://www.davidhbailey.com/dhbpapers/Poissond.pdf.

Samples of minimal polynomials found by PSLQ

k	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 $\exp(8\pi\phi_2(1/32, 1/32))$

$$
\begin{array}{l}
-1 + 21888\alpha + 5893184\alpha^{2} + 15077928064\alpha^{3} - 3696628330464\alpha^{4} - 287791501240448\alpha^{5} - 30287462976198976\alpha^{6} \\
+4426867843186404992\alpha^{7} - 554156920878198587888\alpha^{8} + 10731545733669133574528\alpha^{9} \\
+120048731928709050250048\alpha^{10} + 4376999211577765512726656\alpha^{11} - 279045693458194222125366432\alpha^{12} \\
+18747586287780118903854334848\alpha^{13} - 643310226865188446831485766208\alpha^{14} \\
+120471172259227877284434966655488\alpha^{15} - 117230595100328033884939566091384\alpha^{16} \\
+667772184328316952814362214365568\alpha^{17} - 4130661734713288144037409932696512\alpha^{18} \\
+72313626239383964765274946226530432\alpha^{19} - 1891420571205861612091802761809141088\alpha^{20} \\
+38770881730553471470590641060872686464\alpha^{21} - 577943965397394779947709633563006963008\alpha^{22} \\
+6279796382074485140847650604801614559872\alpha^{23} - 50438907678331243798448849245156136801232\alpha^{24} \\
+305806320133365055812520453224169520739712\alpha^{25} - 1441007171934715336769224848138270812591296\alpha^{26} \\
+5554617356232728647085822946642640269497472\alpha^{27} - 20280024430170705107000630261773759070647328\alpha^{28} \\
+99541720739995105011861264308551867164583808\alpha^{29} - 754081464712315412970559119390477134883548736\alpha^{30} \\
+6271958646895434365874802435136411922022336128\alpha^{31} - 45931349314815625339442690290912948480194150172\alpha^{32} \\
+280907040806572157908285324812126135484630889344\alpha^{33} - 1427273782916972532576299009596755423149111059136\alpha^{34} \\
+6055180299673737231932804443230077408291723908736\alpha^{35} - 21609910939164553316101994301952988793013291135584\alpha^{36} \\
+65433275736596914909292838375737685959952141180288\alpha^{37} - 169928170513492897108417040254326115991438719391296\alpha^{38} \\
+385709310577705218843549196766620216295554031550592\alpha^{39} - 801233230832691550861608914233661767474963249815792\alpha^{40} \\
+1706210557291030772074402183123327251333271061516160\alpha^{41} - 4421210594351357102505784181831242174063263551938496\alpha^{42} \\
+14444199585866329915643888187597383540233619718619776\alpha^{43} - 50968478530199956388487913417905125665738409426112032\alpha^{44} \\
+1698913134549455514927724813351516976839425267825908096\alpha^{45} - 506612996672385619931633440499093959534203673546181440\alpha^{46} \\
+1330573388204326565144545192834096788469932897185696896\alpha^{47} - 3069501638444045841407951432645059776135089489403138888\alpha^{48} \\
+6226636397646752257692349351542872634032398917736673152\alpha^{49} - 11133383491631126059761752734485434504397040890449485504\alpha^{50} \\
+17601823309919260471943648355479182983209248554083752576\alpha^{51} - 24723027443995082126054012492323603544226813344022687712\alpha^{52} \\
+31141043717679289808081270766611355726695735914995681664\alpha^{53} - 35982430389670551550204799905599476866868765647852189248\alpha^{54} \\
+40292583920117898286863491450657424717015372825433076864\alpha^{55} - 48512188214363976290470868896252008979896310883132967248\alpha^{56} \\
+69275112214095149977288310632868535966705567728055958400\alpha^{57} - 114516830148561378617778209682642099604147034577152904128\alpha^{58} \\
+195760470467323759899736578743283333538805684128806803072\alpha^{59} - 317349593507106729834513764473487031789280056911012860320\alpha^{60} \\
+468944248086031450001465269696090117959962662732817675648\alpha^{61} - 622467103741378906100611838210632752408312516281305008960\alpha^{62} \\
+738516443137003178837650661261546833168555909499151978624\alpha^{63} - 781916756680856373187881889706233393197646662361906135622\alpha^{64} \\
+738516443137003178837650661261546833168555909499151978624\alpha^{65} - 622467103741378906100611838210632752408312516281305008960\alpha^{66} \\
+468944248086031450001465269696090117959962662732817675648\alpha^{67} - 317349593507106729834513764473487031789280056911012860320\alpha^{68} \\
+195760470467323759899736578743283333538805684128806803072\alpha^{69} - 114516830148561378617778209682642099604147034577152904128\alpha^{70} \\
+69275112214095149977288310632868535966705567728055958400\alpha^{71} - 48512188214363976290470868896252008979896310883132967248\alpha^{72} \\
+40292583920117898286863491450657424717015372825433076864\alpha^{73} - 35982430389670551550204799905599476866868765647852189248\alpha^{74} \\
+31141043717679289808081270766611355726695735914995681664\alpha^{75} - 24723027443995082126054012492323603544226813344022687712\alpha^{76} \\
+17601823309919260471943648355479182983209248554083752576\alpha^{77} - 11133383491631126059761752734485434504397040890449485504\alpha^{78} \\
+6226636397646752257692349351542872634032398917736673152\alpha^{79} - 3069501638444045841407951432645059776135089489403138888\alpha^{80} \\
+1330573388204326565144545192834096788469932897185696896\alpha^{81} - 506612996672385619931633440499093959534203673546181440\alpha^{82} \\
+1698913134549455514927724813351516976839425267825908096\alpha^{83} - 50968478530199956388487913417905125665738409426112032\alpha^{84} \\
+14444199585866329915643888187597383540233619718619776\alpha^{85} - 4421210594351357102505784181831242174063263551938496\alpha^{86} \\
+1706210557291030772074402183123327251333271061516160\alpha^{87} - 801233230832691550861608914233661767474963249815792\alpha^{88} \\
+385709310577705218843549196766620216295554031550592\alpha^{89} - 169928170513492897108417040254326115991438719391296\alpha^{90} \\
+65433275736596914909292838375737685959952141180288\alpha^{91} - 21609910939164553316101994301952988793013291135584\alpha^{92} \\
+6055180299673737231932804443230077408291723908736\alpha^{93} - 1427273782916972532576299009596755423149111059136\alpha^{94} \\
+280907040806572157908285324812126135484630889344\alpha^{95} - 45931349314815625339442690290912948480194150172\alpha^{96} \\
+6271958646895434365874802435136411922022336128\alpha^{97} - 754081464712315412970559119390477134883548736\alpha^{98} \\
+99541720739995105011861264308551867164583808\alpha^{99} - 20280024430170705107000630261773759070647328\alpha^{100} \\
+5554617356232728647085822946642640269497472\alpha^{101} - 1441007171934715336769224848138270812591296\alpha^{102} \\
+305806320133365055812520453224169520739712\alpha^{103} - 50438907678331243798448849245156136801232\alpha^{104} \\
+6279796382074485140847650604801614559872\alpha^{105} - 577943965397394779947709633563006963008\alpha^{106} \\
+38770881730553471470590641060872686464\alpha^{107} - 1891420571205861612091802761809141088\alpha^{108} \\
+72313626239383964765274946226530432\alpha^{109} - 4130661734713288144037409932696512\alpha^{110} \\
+667772184328316952814362214365568\alpha^{111} - 117230595100328033884939566091384\alpha^{112} \\
+120471172259227877284434966655488\alpha^{113} - 643310226865188446831485766208\alpha^{114} \\
+18747586287780118903854334848\alpha^{115} - 279045693458194222125366432\alpha^{116} \\
+4376999211577765512726656\alpha^{117} + 120048731928709050250048\alpha^{118} + 10731545733669133574528\alpha^{119} \\
-554156920878198587888\alpha^{120} + 4426867843186404992\alpha^{121} - 30287462976198976\alpha^{122} \\
-287791501240448\alpha^{123} - 3696628330464\alpha^{124} + 15077928064\alpha^{125} + 5893184\alpha^{126} + 21888\alpha^{127} - \alpha^{128}
\end{array}
$$

Cautionary example

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

$$\int_0^\infty \cos(2x) \prod_{n=1}^{\infty} \cos(x/n)\, \mathrm{d}x \quad = \quad 0.39269908169872415480783042290993786052464543418723159592 6$$

$$\frac{\pi}{8} \quad = \quad 0.39269908169872415480783042290993786052464617492188822762 1$$

Richard Crandall has shown that this integral is merely the first term of a very rapidly convergent series that converges to $\pi/8$:

$$\frac{\pi}{8} \quad = \quad \sum_{m=0}^{\infty} \int_0^\infty \cos[2(2m+1)x] \prod_{n=1}^{\infty} \cos(x/n)\, \mathrm{d}x$$

1. D.H. Bailey, J.M. Borwein, V. Kapoor and E. Weisstein, “Ten Problems in Experimental Mathematics,” *American Mathematical Monthly*, vol. 113, no. 6 (Jun 2006), pg. 481–409.
2. R.E. Crandall, “Theory of ROOF Walks,” 2007, available at `http://people.reed.edu/~crandall/papers/ROOF.pdf`.

Limitations of *Maple* and *Mathematica*

Maple and *Mathematica* are our first choices whenever symbolic or numeric computations are required. However, both have limitations and bugs.

For example, in a study of Mordell-Tornheim-Witten sums (which arise in mathematical physics), we required high-precision numeric values of derivatives with respect to the order s of polylogarithms:

$$\frac{\partial \mathrm{Li}_s(z)}{\partial s}, \quad \text{where} \quad \mathrm{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s}$$

Maple was not able to numerically evaluate these derivatives at all. *Mathematica*, when asked for 4000 digits, returned only 400 correct digits (at some arguments).

D.H. Bailey, J.M. Borwein and R.E. Crandall, "Computation and theory of extended Mordell-Tornheim-Witten sums," *Mathematics of Computation*, *Ramanujan Journal*, 27 Feb 2013, DOI 10.1007/s11139-012-9427-1, `http://www.davidhbailey.com/dhbpapers/BBC.pdf`.

What is needed for high-precision floating-point software?

- A high-performance, rock-solid-reliable arithmetic engine, with precision scalable to 1,000,000 digits or more.
- A separate package for modest precision (32 and 64 digits)?
- FFT-based multiplication for > 1000 digits.
- A thread-safe design to facilitate multicore parallel processing, and a pathway to extend to graphics processing units (GPUs).
- A comprehensive library of tuned transcendentals: not just sin, cos, exp, etc., but also the gamma function, polylogs (with real and complex arguments), Bessel functions, etc.
- A robust high-level language interface for C++, Fortran-90 and possibly several other languages as well.
- Interfaces for *Maple* and *Mathematica*.

This talk is available at

`http://www.davidhbailey.com/dhbtalks/dhb-pslq.pdf`.