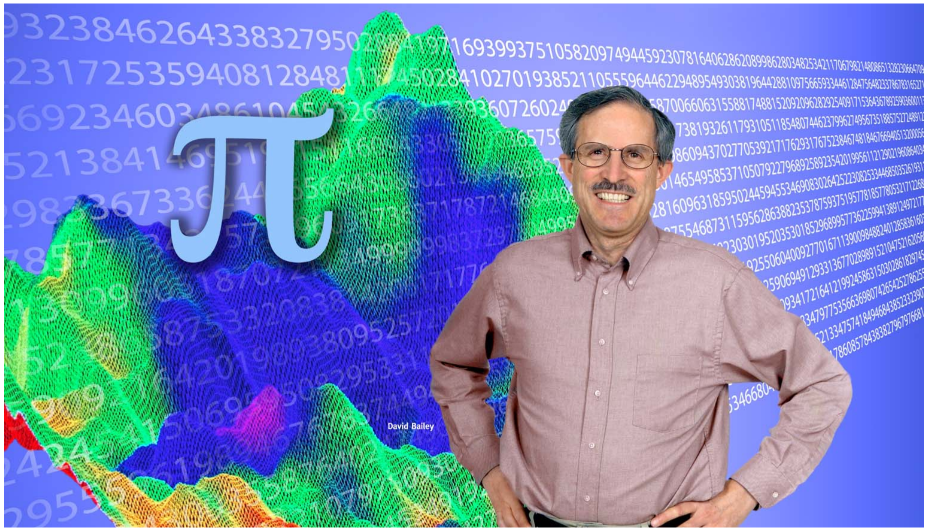
Hand-to-hand combat with thousand-digit integrals

David H Bailey

dhbailey@lbl.gov

Collaborators: Jonathan M. Borwein (University of Newcastle, Australia), Richard Crandall (Apple Computers), numerous others



Analytic evaluation of definite integrals

A frequent theme of experimental mathematics is the recognition of definite integrals in terms of relatively simple closed-form expressions. Such integrals arise in:

- Ising theory of mathematical physics.
- Quantum field theory.
- “Box” integrals (e.g., average distances between points in *n*-cube).
- Random walk theory.

The PSLQ integer relation algorithm

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

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

(or within "epsilon" of zero, where epsilon = 10^{-p} and p is the precision).

At the present time the "PSLQ" algorithm of mathematician-sculptor Helaman Ferguson is the most widely used integer relation algorithm. It was named one of ten "algorithms of the century" by *Computing in Science and Engineering*.

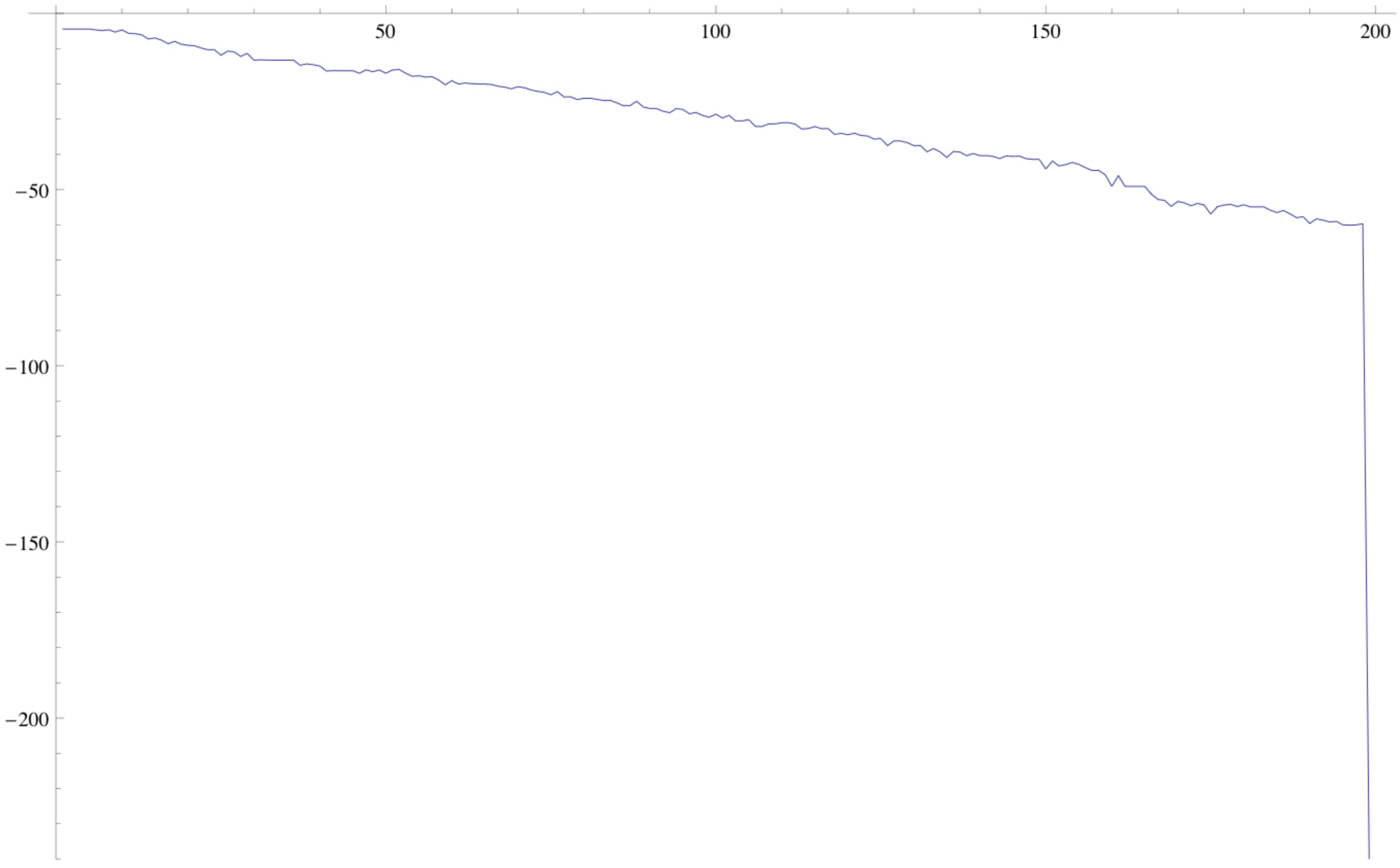
PSLQ (or any other integer relation scheme) requires very high precision (at least n x d digits, where d is the size in digits of the largest a_k), both in the input data and in the operation of the algorithm.

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.

How PSLQ operates

1. PSLQ constructs a sequence of integer-valued matrices B_m that reduces the vector $y = x\, B_m$, until either the relation is found (as one of the columns of B_m), or else precision is exhausted.
2. At the same time, PSLQ generates a steadily growing bound on the size of any possible relation.
3. When a relation is found, the size of smallest entry of the vector y abruptly drops to roughly "epsilon" (i.e. 10^{-p}, where p is the number of digits of precision).
4. The size of this drop can be viewed as a "confidence level" that the relation is real and not merely a numerical artifact -- a drop of 20+ orders of magnitude almost always indicates a real relation.
5. PSLQ (or any other integer relation scheme) requires *very high precision arithmetic*, both in the input data and in the operation of the algorithm:
   - At least nd digits, where n is the dimension, and d is the size in digits of largest a_k.

Decrease of $\log_{10}(\min_k |y_k|)$ as a function of iteration number in a typical PSLQ run



Methodology for using PSLQ to recognize an unknown constant α

1. Calculate α to high precision (e.g., 100 - 1000 digits). This is usually the most expensive step.
2. Make a list of possible terms on the right-hand side (RHS) of a linear formula for α, then calculate each of these *n* terms to the same precision as α.
3. Apply PSLQ to the (n+1)-long vector, using the same numeric precision as α.
4. When PSLQ runs, look for a sharp drop (at least 20 orders of magnitude) in the size of the reduced *y* vector by, to a value near "epsilon."
5. If no credible relation is found, try expanding the list of RHS terms.

Some related approaches:

1. If you suspect α is algebraic of degree *n* (the root of a degree-*n* polynomial with integer coefficients), apply PSLQ to the (n+1)-long vector $(1, \alpha, \alpha^2, \alpha^3, \ldots, \alpha^n)$.
2. If you suspect α is given by a multiplicative relation, take logarithms of α and the list of constants, then apply PSLQ to the (n+1)-long vector.

Gaussian quadrature

Gaussian quadrature is often the most efficient scheme for regular functions (including at endpoints) and modest precision (< 1000 digits):

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \quad \approx \quad \sum_{j=1}^{n} w_j f(x_j)$$

The abscissas (x_j) are the roots of the n-th degree Legendre polynomial $P_n(x)$ on [-1,1]. The weights (w_j) are given by

$$w_j \quad = \quad \frac{-2}{(n+1)P_n'(x_j)P_{n+1}(x_j)}$$

The abscissas (x_j) are computed by Newton iterations, with starting values cos[π(j-1/4)/(n+1/2)]. Legendre polynomials and their derivatives can be computed using the formulas $P_0(x) = 0$, $P_1(x) = 1$,

$$\begin{aligned} (k+1)P_{k+1}(x) &= (2k+1)xP_k(x) - kP_{k-1}(x) \\ P_n'(x) &= n(xP_n(x) - P_{n-1}(x))/(x^2 - 1) \end{aligned}$$

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.

The Euler-Maclaurin formula of numerical analysis

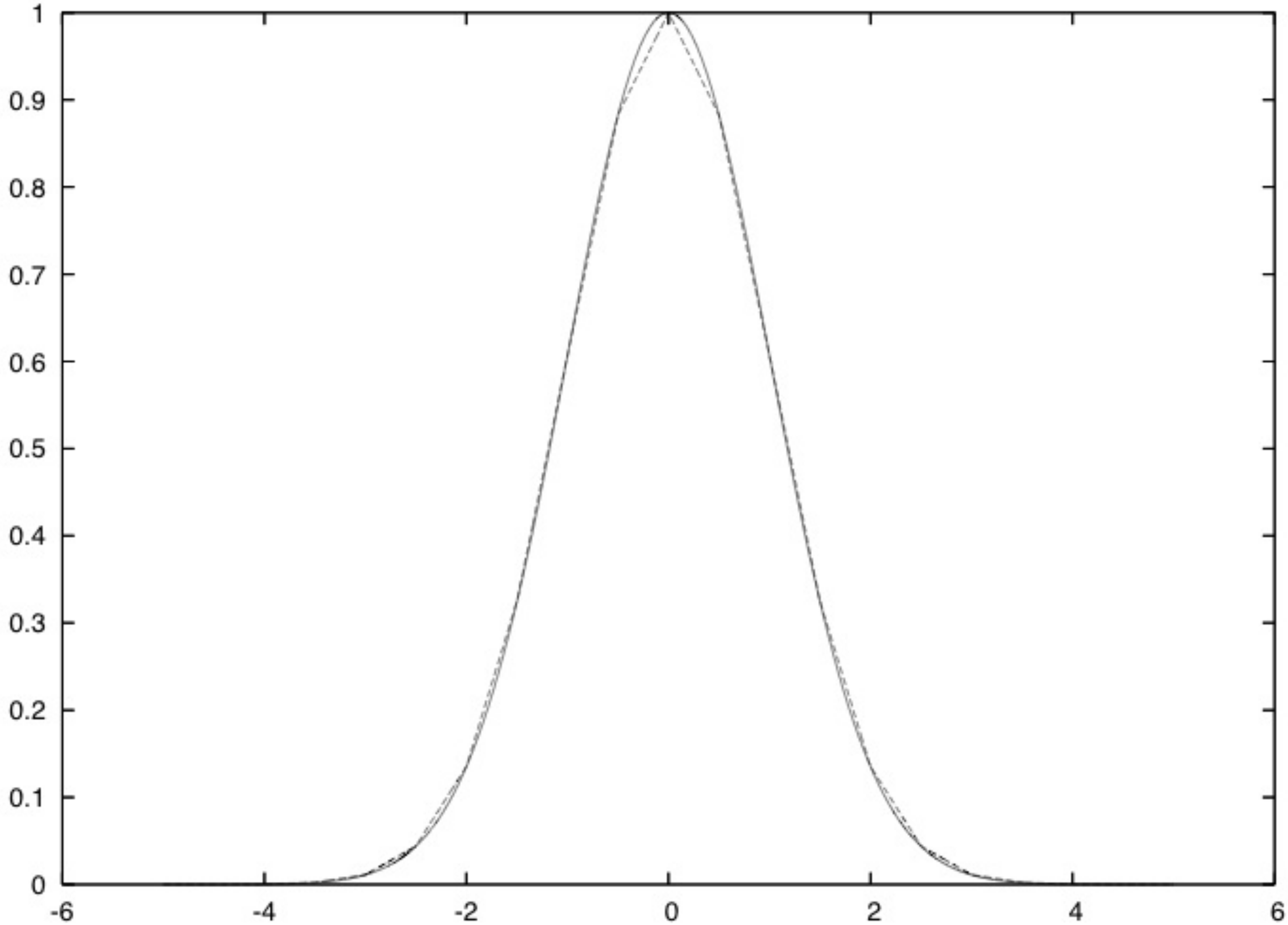
$$
\begin{aligned}
\int_a^b f(x)\,\mathrm{d}x &= h\sum_{j=0}^{n} f(x_j) - \frac{h}{2}(f(a)+f(b)) \\
&\quad - \sum_{i=1}^{m} \frac{h^{2i}B_{2i}}{(2i)!}\left(D^{2i-1}f(b) - D^{2i-1}f(a)\right) - E(h) \\
|E(h)| &\leq 2(b-1)(h/(2\pi))^{2m+2} \max_{a\le x\le b} |D^{2m+2}f(x)|
\end{aligned}
$$

Here $h = (b - a)/n$ and $x_j = a + jh$; B_{2i} are Bernoulli numbers; $D^m f(x)$ is the m-th derivative of $f(x)$. The E-M formula can be thought of as providing high-order correction terms to the trapezoidal rule.

Note when $f(x)$ and all of its derivatives are zero at the endpoints a and b (as in a bell-shaped curve), the error $E(h)$ of a simple trapezoidal approximation to the integral goes to zero more rapidly than any power of h.

K. Atkinson, *An Introduction to Numerical Analysis*, John Wiley, 1989, pg. 289.

Trapezoidal approximation to a bell-shaped function



Tanh-sinh quadrature

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

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

where $x_j = g(hj)$ and $w_j = g'(hj)$. The x_j and w_j can be precomputed.

Since $g'(t)$ goes to zero very rapidly for large t, the integrand $f(g(t))\,g'(t)$ typically is a nice bell-shaped function for which the Euler-Maclaurin formula implies that the simple summation above is remarkably accurate. 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. It is also best at very high precision (> 1000 digits), because the computation of abscissas and weights is much faster than with Gaussian quadrature or other schemes.

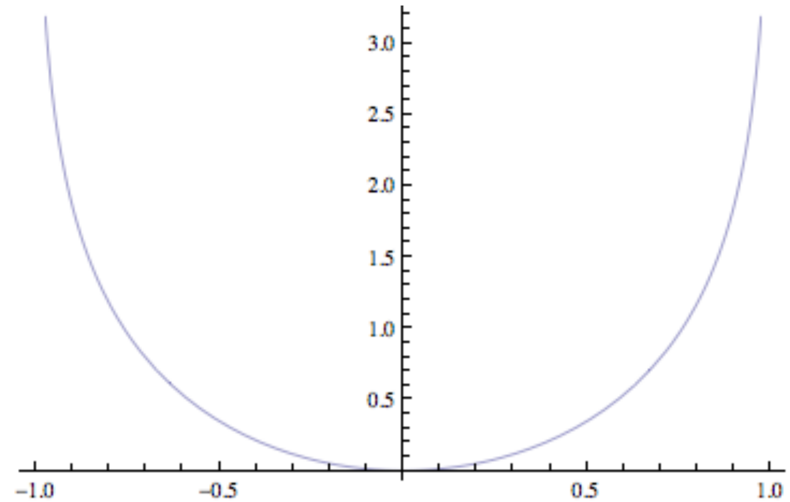
1. D.H. Bailey, X.S. Li and K. Jeyabalan, "A comparison of three high-precision quadrature schemes," *Experimental Mathematics*, vol. 14 (2005), no. 3, pg. 317-329.
2. H. Takahasi and M. Mori, "Double exponential formulas for numerical integration," Publications of RIMS, Kyoto University, vol. 9 (1974), pg. 721–741.

Original and transformed integrand functions

Original integrand function on [-1,1]:

$$f(x) = -\log\cos\left(\frac{\pi x}{2}\right)$$

Note the singularities at the endpoints.

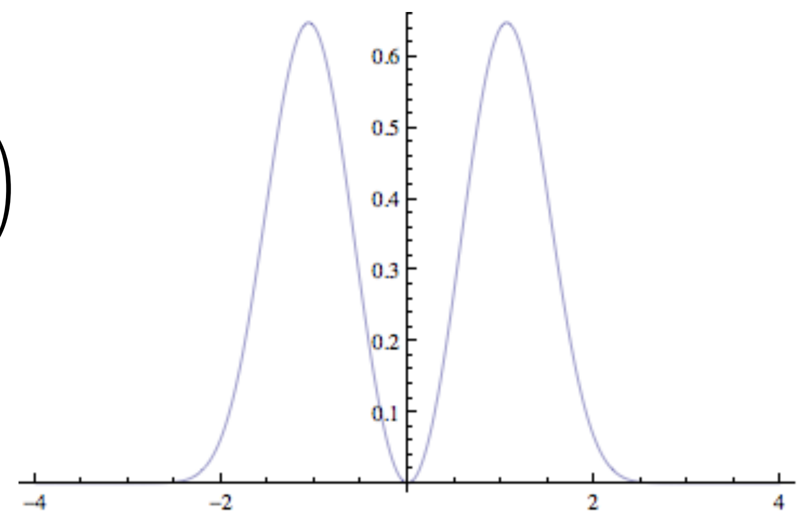


Transformed using $x = g(t) = \tanh(\sinh t)$:

$$f(g(t))g'(t) \quad =$$

$$-\log\cos[\pi/2\cdot\tanh(\sinh t)]\left(\frac{\cosh(t)}{\cosh(\sinh t)^2}\right)$$

This is now a nice smooth bell-shaped function, so the E-M formula implies that a trapezoidal approximation is very accurate.



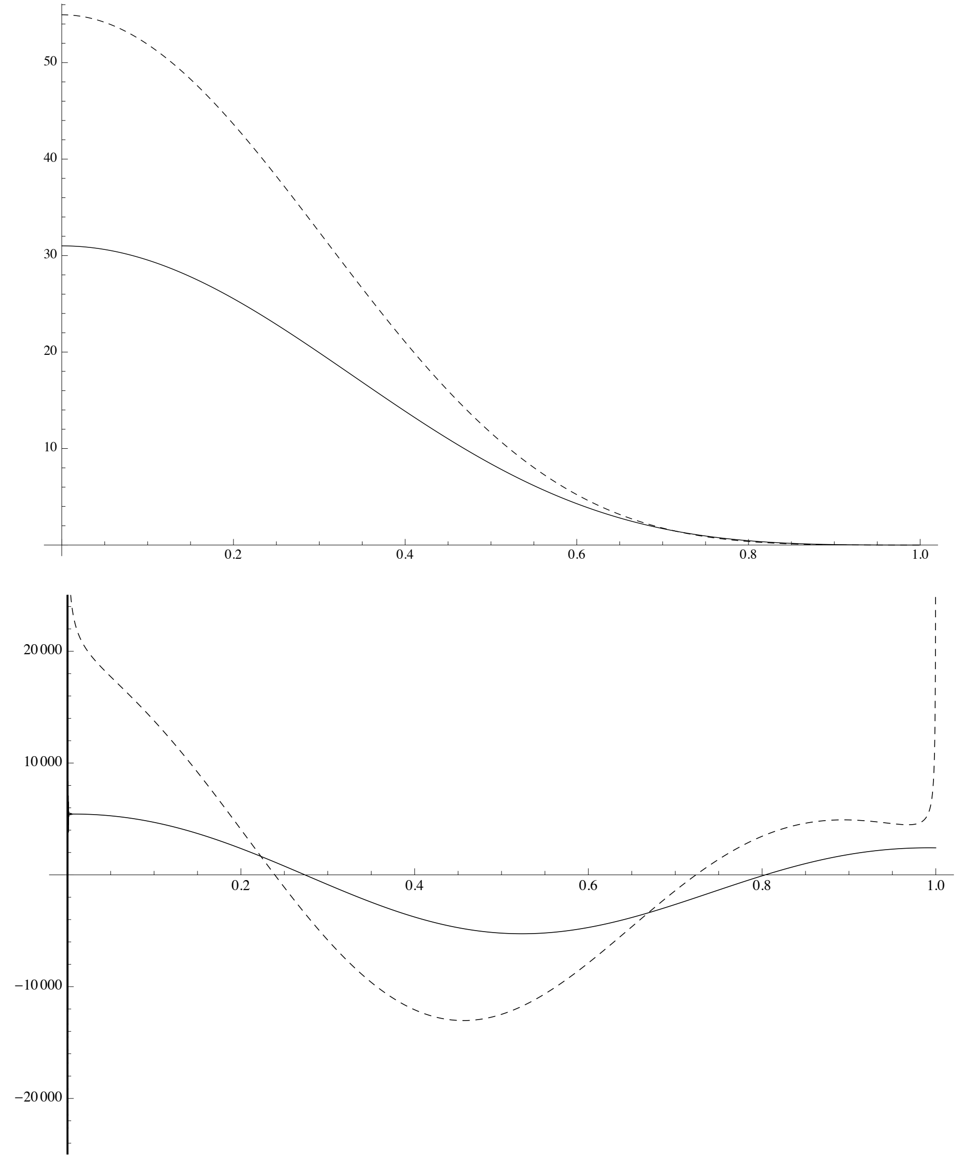
Regular function or not?

Plots of $f(x) = \sin^p(\pi x)\, \zeta(p,x)$ (upper) and its fourth derivative (lower), for $p = 3$ (solid) and $p = 3.5$ (dashed). Here ζ is Hurwitz zeta function.

When $p = 3.5$, the function itself appears completely regular, but the fourth derivative blows up at both endpoints.

As a result, Gaussian quadrature works very poorly for this function.

But tanh-sinh works fine.



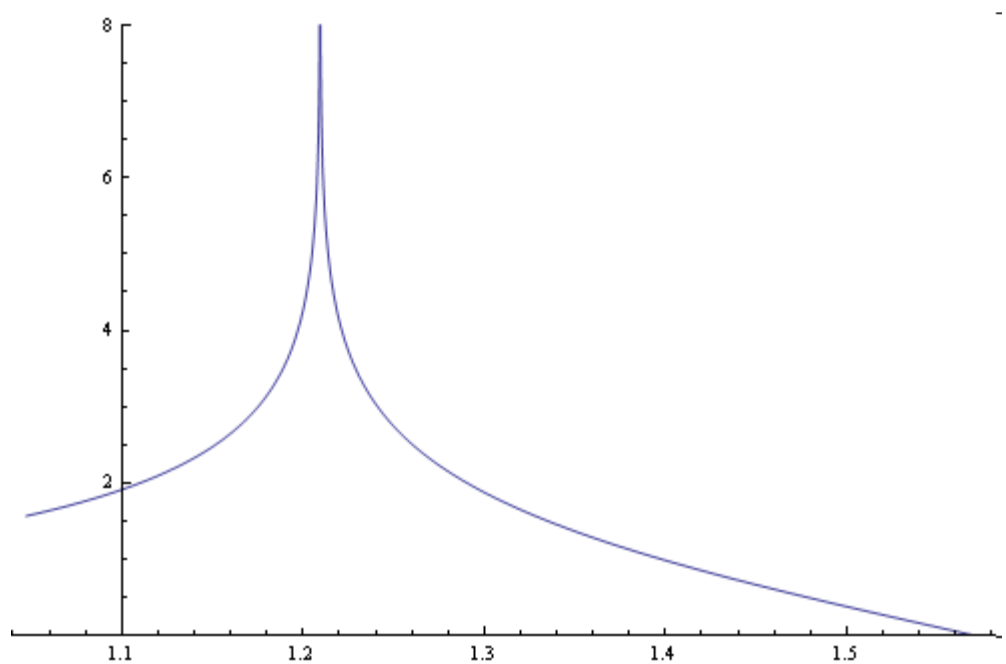
A log-tan integral identity verified with tanh-sinh quadrature

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| \mathrm{d}t \quad = \quad L_{-7}(2) \quad =$$

$$\sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2} \right]$$

This identity arises from analysis of volumes of knot complements in hyperbolic space. This is simplest of 998 related identities.

We verified this numerically to 20,000 digits, using tanh-sinh quadrature on a highly parallel computer. A proof was known, but we weren't aware of this at the time.



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 .

Integration of oscillatory functions on semi-infinite intervals

- Many functions on a semi-infinite interval can be computed using Gaussian or tanh-sinh quadrature by a simple change of variable – i.e., for integrals on [1, infinity), use the transformation $u = 1/t$.
- Oscillatory functions on semi-infinite intervals are more challenging -- even tanh-sinh fails for many such integrals.
- Some oscillatory integrals involving sin or cos can be handled using a technique due to Ooura and Mori.
- For oscillatory integrals involving Bessel functions, we have used a scheme due to Sidi, Lucas and Sloane: Divide integral into intervals $[n\pi, (n+1)\pi]$ and then use Sidi's mW scheme to extrapolate the value of infinite sum.

1. S.K. Lucas and H.A. Stone, "Evaluating infinite integrals involving Bessel functions of arbitrary order," *Journal of Computational and Applied Mathematics*, vol. 64 (1995), pg. 217-231.
2. T. Ooura and M. Mori, "Double exponential formulas for oscillatory functions over the half infinite interval," *Journal of Computational and Applied Mathematics*, vol. 38 (1991), pg. 353-360.

Ising integrals from mathematical physics

We recently applied our methods to study three classes of integrals that arise in the Ising theory of mathematical physics – D_n and two others:

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

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

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

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

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.

Computing and evaluating C_n

We observed that the multi-dimensional C_n integrals can be transformed to 1-D integrals:

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

where K_0 is the modified Bessel function. In this form, the C_n constants appear naturally in in quantum field theory (QFT).

We used this formula to compute 1000-digit numerical values of various C_n, from which the following results and others were found, then proven:

$$\begin{aligned} C_1 &= 2 \\ C_2 &= 1 \\ C_3 &= \mathrm{L}_{-3}(2) = \sum_{n \geq 0} \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right) \\ C_4 &= \frac{7}{12} \zeta(3) \end{aligned}$$

Limiting value of C_n: What is this number?

The C_n numerical values appear to approach a limit. For instance,

$$C_{1024} = 0.63047350337438679612204019271087890435458707871273234\ldots$$

What is this limit? We copied the first 50 digits of this numerical value into the online Inverse Symbolic Calculator (ISC):
http://isc.carma.newcastle.edu.au

The result was:

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

where gamma denotes Euler's constant. Finding this limit led us to the asymptotic expansion and made it clear that the integral representation of C_n is fundamental.

Other Ising integral evaluations found using high-precision 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 $\mathrm{Li}_n(x)$ is the polylog function.

D_2, D_3 and D_4 were originally provided to us by mathematical physicist 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 this extremely complicated 3-D integral:

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 this question.

$$
\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 QFT for odd *k*):

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

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

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

Similar, but more complicated, recursions have been found for all *n*.

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.

J.M. Borwein and B. Salvy, “A proof of a recursion for Bessel moments,” *Experimental Mathematics*, vol. 17 (2008), pg. 223-230.

Four hypergeometric evaluations

$$c_{3,0} = \frac{3\Gamma^6(1/3)}{32\pi 2^{2/3}} = \frac{\sqrt{3}\pi^3}{8}\,{}_3F_2\left(\begin{array}{c}1/2,1/2,1/2\\1,1\end{array}\middle|\frac{1}{4}\right)$$

$$c_{3,2} = \frac{\sqrt{3}\pi^3}{288}\,{}_3F_2\left(\begin{array}{c}1/2,1/2,1/2\\2,2\end{array}\middle|\frac{1}{4}\right)$$

$$c_{4,0} = \frac{\pi^4}{4}\sum_{n=0}^{\infty}\frac{\binom{2n}{n}^4}{4^{4n}} = \frac{\pi^4}{4}\,{}_4F_3\left(\begin{array}{c}1/2,1/2,1/2,1/2\\1,1,1\end{array}\middle|1\right)$$

$$c_{4,2} = \frac{\pi^4}{64}\left[4\,{}_4F_3\left(\begin{array}{c}1/2,1/2,1/2,1/2\\1,1,1\end{array}\middle|1\right) - 3\,{}_4F_3\left(\begin{array}{c}1/2,1/2,1/2,1/2\\2,1,1\end{array}\middle|1\right)\right] - \frac{3\pi^2}{16}$$

D.H. Bailey, J.M. Borwein, D.M. Broadhurst and M.L. Glasser, “Elliptic integral representation of Bessel moments,” *Journal of Physics A: Mathematical and Theoretical*, vol. 41 (2008), 5203-5231.

2-D integral in Bessel moment study

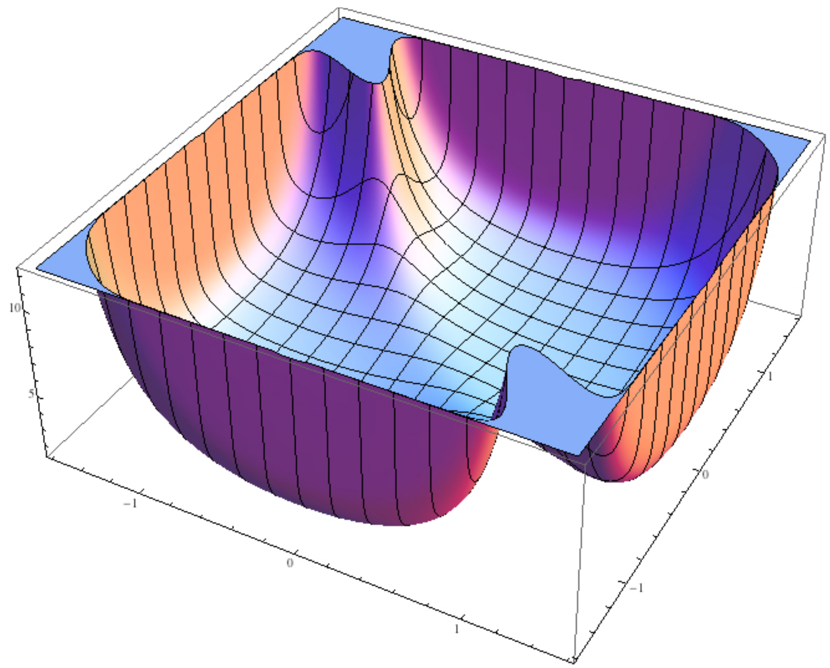
We conjectured (and later proved)

$$c_{5,0} \quad = \quad \frac{\pi}{2} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \frac{\mathbf{K}(\sin\theta)\,\mathbf{K}(\sin\phi)}{\sqrt{\cos^2\theta\cos^2\phi + 4\sin^2(\theta+\phi)}}\, d\theta\, d\phi$$

Here **K** denotes the complete elliptic integral of the first kind

Note that the integrand function has singularities on all four sides of the region of integration.

We were able to evaluate this integral to 120-digit accuracy, using 1024 cores of the "Franklin" Cray XT4 system at LBNL.



Box integrals

The following integrals appear in numerous arenas of math and physics:

$$B_n(s) \;\; := \;\; \int_0^1 \cdots \int_0^1 \left(r_1^2 + \cdots + r_n^2\right)^{s/2} \, dr_1 \cdots dr_n$$

$$\Delta_n(s) \;\; := \;\; \int_0^1 \cdots \int_0^1 \left((r_1 - q_1)^2 + \cdots + (r_n - q_n)^2\right)^{s/2} \, dr_1 \cdots dr_n \, dq_1 \cdots dq_n$$

- $B_n(1)$ is the expected distance of a random point from the origin of *n*-cube.
- $\Delta_n(1)$ is the expected distance between two random points in *n*-cube.
- $B_n(-n+2)$ is the expected electrostatic potential in an *n*-cube whose origin has a unit charge.
- $\Delta_n(-n+2)$ is the expected 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.

One example result

$$\Delta_3(-1) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{(-1 + e^{-u^2} + \sqrt{\pi}\, u \operatorname{erf}(u))^3}{u^6}\, \mathrm{d}u$$

$$= \frac{1}{15}\left(6 + 6\sqrt{2} - 12\sqrt{3} - 10\pi + 30\log(1+\sqrt{2}) + 30\log(2+\sqrt{3})\right)$$

As in many of the previous results, this was found by first computing the integral to high precision (250 to 1000 digits), conjecturing possible terms on the right-hand side, then applying PSLQ to look for a relation. We now have proven this result.

Dozens of similar results have since been found (see next few viewgraphs), raising hope that all box integrals eventually will be evaluated in closed form.

D.H. Bailey, J.M. Borwein and R.E. Crandall, “Advances in the theory of box integrals,” *Mathematics of Computation*, vol. 79, no. 271 (Jul 2010), pg. 1839-1866; http://crd.lbl.gov/~dhbailey/dhbpapers/BoxII.pdf.

Recent 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	$-3\mathrm{G} + \frac{3}{2}\pi\log(1+\sqrt{2}) + 3\ \mathrm{Ti}_2(3-2\sqrt{2})$
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.

Recent evaluations of box integrals, continued

n	s	$B_n(s)$
4	-5	$-\sqrt{8}\ \arctan\left(\frac{1}{\sqrt{8}}\right)$
4	-3	$4\ G - 12\,\mathrm{Ti}_2(3-2\sqrt{2})$
4	-2	$\pi\ \log\left(2+\sqrt{3}\right) - 2\,G - \frac{\pi^2}{8}$
4	-1	$2\log 3 - \frac{2}{3}\,G + 2\,\mathrm{Ti}_2\left(3-2\,\sqrt{2}\right) - \sqrt{8}\ \arctan\left(\frac{1}{\sqrt{8}}\right)$
4	1	$\frac{2}{5} - \frac{G}{10} + \frac{3}{10}\,\mathrm{Ti}_2\left(3-2\sqrt{2}\right) + \log 3 - \frac{7\sqrt{2}}{10}\ \arctan\left(\frac{1}{\sqrt{8}}\right)$
5	-3	$-\frac{110}{9}\,G - 10\ \log\left(2-\sqrt{3}\right)\ \theta - \frac{1}{8}\,\pi^2 + 5\ \log\left(\frac{1+\sqrt{5}}{2}\right) - \frac{5}{2}\,\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right)$ $-10\,\mathrm{Cl}_2\left(\frac{1}{3}\,\theta+\frac{1}{3}\,\pi\right) + 10\,\mathrm{Cl}_2\left(\frac{1}{3}\,\theta-\frac{1}{6}\,\pi\right)$ $+\frac{10}{3}\,\mathrm{Cl}_2\left(\theta+\frac{1}{6}\,\pi\right) + \frac{20}{3}\,\mathrm{Cl}_2\left(\theta+\frac{4}{3}\,\pi\right) - \frac{10}{3}\,\mathrm{Cl}_2\left(\theta+\frac{5}{3}\,\pi\right) - \frac{20}{3}\,\mathrm{Cl}_2\left(\theta+\frac{11}{6}\,\pi\right)$
5	-2	$\frac{8}{3}\,B_5(-6) - \frac{1}{3}\,B_5(-4) + \frac{5}{2}\,\pi\log(3) + 10\,\mathrm{Ti}_2\left(\frac{1}{3}\right) - 10\,G$
5	-1	$-\frac{110}{27}\,G + \frac{10}{3}\ \log\left(2-\sqrt{3}\right)\ \theta + \frac{1}{48}\,\pi^2 + 5\ \log\left(\frac{1+\sqrt{5}}{2}\right) - \frac{5}{2}\,\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right)$ $+\frac{10}{3}\,\mathrm{Cl}_2\left(\frac{1}{3}\,\theta+\frac{1}{3}\,\pi\right) - \frac{10}{3}\,\mathrm{Cl}_2\left(\frac{1}{3}\,\theta-\frac{1}{6}\,\pi\right)$ $-\frac{10}{9}\,\mathrm{Cl}_2\left(\theta+\frac{1}{6}\,\pi\right) + \frac{20}{3}\,\mathrm{Cl}_2\left(\theta+\frac{4}{3}\,\pi\right) - \frac{10}{3}\,\mathrm{Cl}_2\left(\theta+\frac{5}{3}\,\pi\right) + \frac{20}{9}\,\mathrm{Cl}_2\left(\theta+\frac{11}{6}\,\pi\right)$
5	1	$-\frac{77}{81}\,G + \frac{7}{9}\ \log\left(2-\sqrt{3}\right)\ \theta + \frac{1}{360}\,\pi^2 + \frac{1}{6}\,\sqrt{5} + \frac{10}{3}\ \log\left(\frac{1+\sqrt{5}}{2}\right) - \frac{4}{3}\,\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right) +$ $\frac{7}{9}\,\mathrm{Cl}_2\left(\frac{1}{3}\,\theta+\frac{1}{3}\,\pi\right) - \frac{7}{9}\,\mathrm{Cl}_2\left(\frac{1}{3}\,\theta-\frac{1}{6}\,\pi\right)$ $-\frac{7}{27}\,\mathrm{Cl}_2\left(\theta+\frac{1}{6}\,\pi\right) - \frac{14}{27}\,\mathrm{Cl}_2\left(\theta+\frac{4}{3}\,\pi\right) + \frac{7}{27}\,\mathrm{Cl}_2\left(\theta+\frac{5}{3}\,\pi\right) + \frac{14}{27}\,\mathrm{Cl}_2\left(\theta+\frac{11}{6}\,\pi\right)$

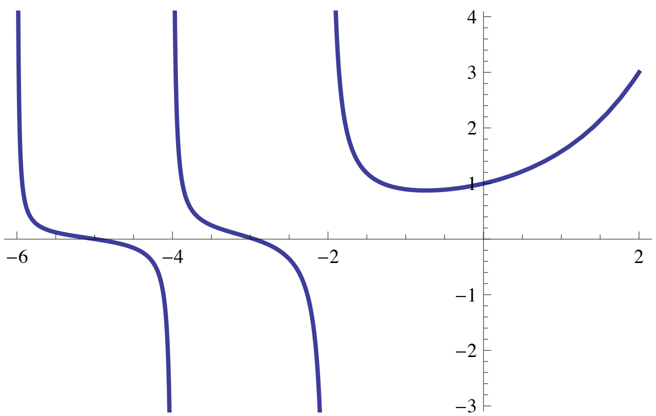
Here *G* is Catalan; Cl is Clausen function; Ti is Lewin function; and θ = arctan((16-3*sqrt(15))/11).

Ramble integrals

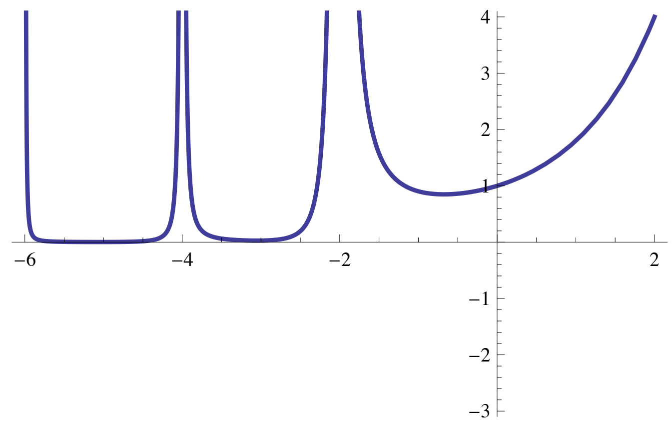
Continuing some earlier research [see refs below], we consider

$$W_n(s) \quad = \quad \int_{[0,1]^n} \left| \sum_{k=1}^{n} e^{2\pi x_k i}, \right|^s \mathrm{d}x$$

which is the *s*-th moment of the distance to the origin after *n* steps of a uniform random walk in the plane, with unit steps in a random direction.



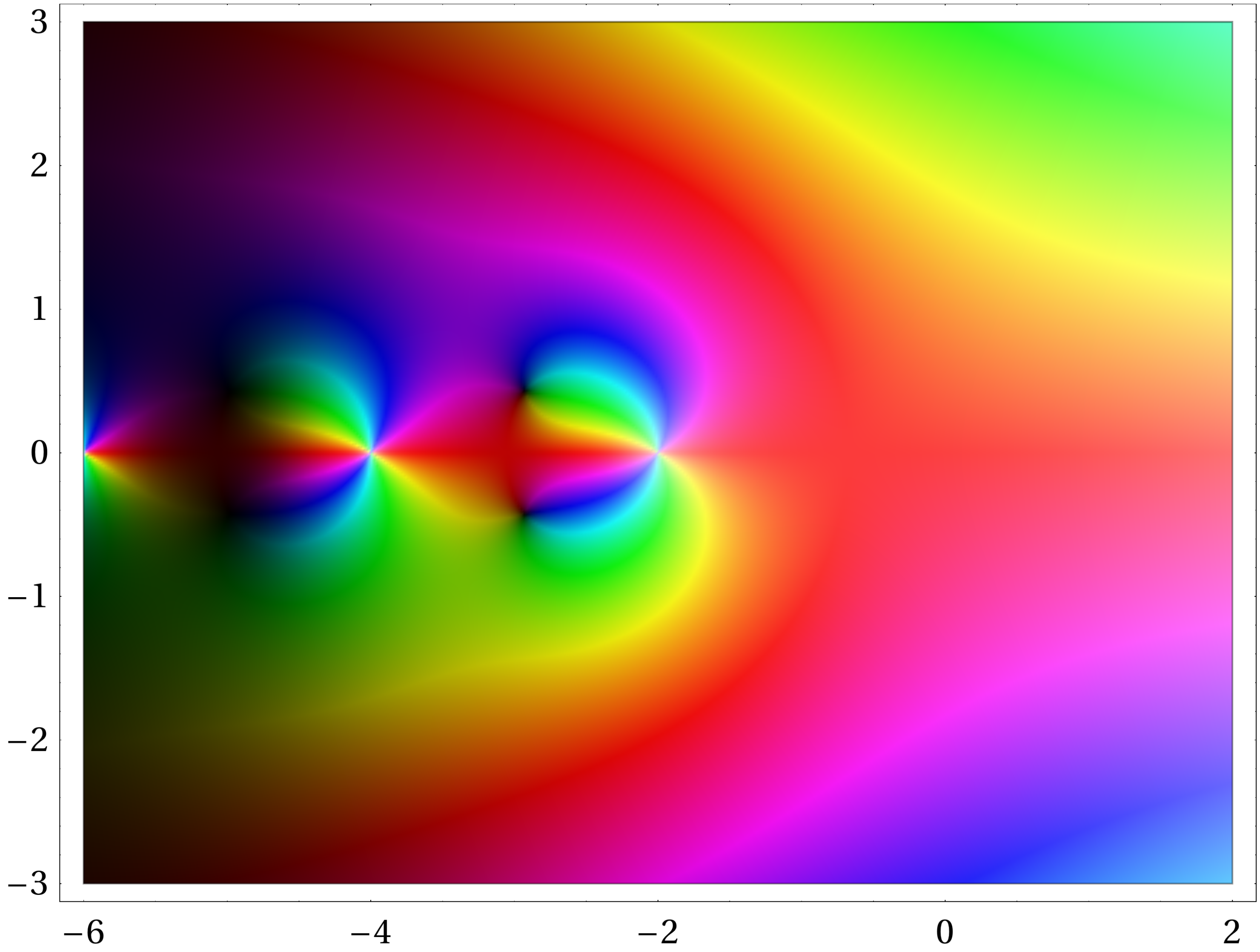
W_3



W_4

1. J.M. Borwein, D. Nuyens, A. Straub and J. Wan, “Some arithmetic properties of short random walk integrals,” *Ramanujan Journal*, to appear, available at http://www.carma.newcastle.edu.au/~jb616/walks.pdf.
2. J.M. Borwein, A. Straub, and J. Wan, “Three-step and four-step random walk integrals,” *Experimental Mathematics*, to appear, available at http://www.carma.newcastle.edu.au/~jb616/walks2.pdf.

Complex plane graph of W_4



Some results

$$
\begin{aligned}
W_3'(0) &= \int_{1/6}^{5/6} \log(2\sin(\pi y))\mathrm{d}y \;=\; \frac{1}{\pi}\,\mathrm{Cl}\left(\frac{\pi}{3}\right) \\
W_3'(2) &= 2 + \frac{3}{\pi}\mathrm{Cl}\left(\frac{\pi}{3}\right) - \frac{3\sqrt{3}}{2\pi} \\
W_4'(0) &= \frac{7}{2}\frac{\zeta(3)}{\pi^2} \\
W_n'(0) &= \log(2) - \gamma - \int_0^1 \left(J_0^n(x) - 1\right)\frac{\mathrm{d}x}{x} - \int_1^\infty J_0^n(x)\frac{\mathrm{d}x}{x} \\
&= \log(2) - \gamma - n\int_0^\infty \log(x) J_0^{n-1}(x) J_1(x)\mathrm{d}x \\
W_n''(0) &= n\int_0^\infty \left(\log\left(\frac{2}{x}\right) - \gamma\right)^2 J_0^{n-1}(x) J_1(x)\mathrm{d}x \\
W_n'(-1) &= (\log 2 - \gamma)W_n(-1) - \int_0^\infty \log(x) J_0^n(x)\mathrm{d}x \\
W_n'(1) &= \int_0^\infty \frac{n}{x} J_0^{n-1}(x) J_1(x)\left(1 - \gamma - \log(2x)\right)\mathrm{d}x
\end{aligned}
$$

Here Cl denotes the Clausen function and gamma denotes Euler’s constant.

1000-digit computations of $W_n'(0)$ using Sidi's scheme for oscillating functions

n	Precision	Iterations	Time	30-digit numerical values
3	200	159	123	0.323065947219450514093636510723$8\ldots$
	400	320	2046	
	1000	802	106860	
5	200	159	249	0.544412561752185585195878062745$0\ldots$
	400	319	2052	
	1000	801	106860	
7	200	157	249	0.702926292476967266787823944395$2\ldots$
	400	318	2050	
	1000	800	106860	
9	200	156	248	0.824156239532388694820522824849$6\ldots$
	400	317	2120	
	1000	799	106800	
11	200	155	247	0.921850886732653697565891527970$3\ldots$
	400	316	4123	
	1000	796	213480	
13	200	154	246	1.003583530489320110604453874320$8\ldots$
	400	314	4113	
	1000	796	213540	
15	200	152	245	1.073826217256856036184252781500$3\ldots$
	400	313	4096	
	1000	795	213480	
17	200	151	244	1.135410703767411072953239250042$9\ldots$
	400	312	4104	
	1000	794	213360	

For the even-*n* case, even Sidi's scheme doesn't work. We have 50 digits, though.

Elliptic function integrals

The research with ramble integrals led us to study integrals of the form:

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

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

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

James Wan, "Moments of products of elliptic integrals," *Advances in Applied Mathematics*, vol. 48 (2012), available at http://carma.newcastle.edu.au/jamesw/mkint.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 <= 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. For example:

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

Summary of EE'KK' integral results

D_1	D_2	Relations	Basis	Total	Precision	Basis norm bound	Max relation norm
0	1	1	3	4	1500	1.582082×10^{298}	2.236068×10^{0}
1	1	5	3	8	1500	2.155768×10^{297}	3.605551×10^{0}
2	1	9	3	12	1500	2.155768×10^{297}	5.916080×10^{0}
3	1	13	3	16	1500	2.155768×10^{297}	1.679286×10^{1}
4	1	17	3	20	1500	2.155768×10^{297}	6.592420×10^{1}
5	1	21	3	24	1500	2.155768×10^{297}	2.419628×10^{2}
0	2	4	6	10	1500	5.609665×10^{261}	2.109502×10^{1}
1	2	12	8	20	1500	4.877336×10^{196}	5.744563×10^{0}
2	2	22	8	30	1500	6.109876×10^{195}	2.293469×10^{1}
3	2	32	8	40	1500	6.109876×10^{195}	2.293469×10^{1}
4	2	42	8	50	1500	6.109876×10^{195}	1.639153×10^{3}
5	2	52	8	60	1500	6.109876×10^{195}	2.428260×10^{3}
0	3	14	6	20	1500	3.871282×10^{262}	2.664001×10^{2}
1	3	34	6	40	1500	2.164052×10^{261}	8.960469×10^{1}
2	3	52	8	60	1500	1.496420×10^{197}	9.666276×10^{2}
3	3	72	8	80	1500	2.829003×10^{196}	2.291372×10^{3}
4	3	92	8	100	1500	8.853827×10^{195}	5.860112×10^{3}
5	3	112	8	120	1500	8.853827×10^{195}	9.240898×10^{4}
0	4	20	15	35	1500	2.689124×10^{104}	1.963656×10^{4}
1	4	53	17	70	1500	6.195547×10^{91}	2.186030×10^{3}
2	4	88	17	105	1500	4.059577×10^{91}	2.970026×10^{4}
3	4	121	19	140	1500	8.856138×10^{81}	5.658994×10^{5}
4	4	156	19	175	1500	2.759846×10^{82}	5.571466×10^{6}
5	4	191	19	210	1500	1.663418×10^{82}	1.857555×10^{5}
0	5	45	11	56	1500	1.256977×10^{142}	1.061532×10^{5}
1	5	101	11	112	1500	2.602478×10^{142}	1.025453×10^{5}
2	5	155	13	168	1500	2.151577×10^{120}	3.953731×10^{5}
3	5	211	13	224	1500	1.314945×10^{120}	3.728547×10^{5}
4	5	265	15	280	1500	5.040597×10^{104}	8.658997×10^{6}
5	5	321	15	336	1500	4.186191×10^{104}	3.954175×10^{11}
0	6	56	28	84	3000	2.958413×10^{105}	1.748907×10^{6}
1	6	138	30	168	3000	2.018080×10^{98}	2.219430×10^{6}
2	6	222	30	252	3000	3.089318×10^{98}	6.301251×10^{8}
3	6	304	32	336	3000	1.324953×10^{92}	2.929549×10^{10}
4	6	388	32	420	3000	9.312061×10^{91}	6.168516×10^{12}
5	6	470	34	504	3000	6.616755×10^{86}	7.199329×10^{13}

For additional details

David H. Bailey and Jonathan M. Borwein, “Hand-to-hand combat with thousand-digit integrals,” *Journal of Computational Science*, vol. 3 (2012), pg. 77-86, preprint available at:

`http://crd.lbl.gov/~dhbailey/dhbpapers/combat.pdf`

Fractal box integrals

- The box integral work, when applied to mouse brains, has suggested extensions to integrals over Cantor sets (1-D, 2-D and 3-D). Some interesting new results have been obtained:
  - David H. Bailey, Jonathan M. Borwein, Richard E. Crandall and Michael G. Rose, “Expectations on fractal sets,” manuscript, 22 Aug 2012, available at http://crd-legacy.lbl.gov/~dhbailey/dhbpapers/fracboxes.pdf.
- The fractal set computations were mostly done using Monte Carlo methods. Can truly high-precision numerical values be obtained?
  - Jon Borwein and Andrew Mattingtly (IBM Australia) have just completed some results to 12+ digits.

Computations of box integrals on Cantor sets – analytic vs numeric

P	$\delta(C_1(P))$	$B(2, C_1(P))$			$\Delta(2, C_1(P))$		
	Decimal	Rational	Decimal	Numeric	Rational	Decimal	Numeric
0	0.630930	3/8	0.375000	0.375013	1/4	0.250000	0.250009
0001	0.723197	7379/19680	0.374949	0.374941	2459/9840	0.249898	0.249904
0010	0.723197	2457/6560	0.374543	0.374543	817/3280	0.249085	0.249080
0100	0.723197	2433/6560	0.370884	0.370887	793/3280	0.241768	0.241765
1000	0.723197	2217/6560	0.337957	0.337937	577/3280	0.175915	0.175928
001	0.753953	409/1092	0.374542	0.374552	68/273	0.249084	0.249092
010	0.753953	135/364	0.370879	0.370877	22/91	0.241758	0.241751
100	0.753953	123/364	0.337912	0.337895	16/91	0.175824	0.175824
0011	0.815465	737/1968	0.374492	0.374486	245/984	0.248984	0.248989
01	0.815465	89/240	0.370833	0.370836	29/120	0.241667	0.241661
0110	0.815465	243/656	0.370427	0.370429	79/328	0.240854	0.240850
10	0.815465	27/80	0.337500	0.337481	7/40	0.175000	0.175014
1001	0.815465	665/1968	0.337907	0.337894	173/984	0.175813	0.175812
1100	0.815465	219/656	0.333841	0.333825	55/328	0.167683	0.167686
011	0.876977	809/2184	0.370421	0.370397	263/1092	0.240842	0.240847
101	0.876977	737/2184	0.337454	0.337442	191/1092	0.174908	0.174904
110	0.876977	243/728	0.333791	0.333781	1/6	0.167582	0.167583
0111	0.907732	7289/19680	0.370376	0.370350	2369/9840	0.240752	0.240757
1011	0.907732	6641/19680	0.337449	0.337440	1721/9840	0.174898	0.174903
1101	0.907732	6569/19680	0.333791	0.333765	1649/9840	0.167581	0.167574
1110	0.907732	2187/6560	0.333384	0.333386	547/3280	0.166768	0.166774
1	1.000000	1/3	0.333333	0.333333	1/6	0.166667	0.166671
Max error				0.000033			0.000026
RMS error				0.000014			0.000008

Open questions and future directions

- Sidi has proposed a new algorithm for integrating even-order Bessel function integrals. Does someone want to try it?
- In general, can we extend fast numerical schemes such as Gaussian quadrature, tanh-sinh quadrature and Sidi's algorithms for oscillating functions to more general domains, such as Cantor sets?
- Even with the tanh-sinh and highly parallel computer systems, 20,000 digits are the most we can compute in reasonable time for 1-D integrals. Are there any fundamentally faster methods?
- 2-D, 3-D and higher integrals are extremely expensive – much more so than 1-D. Are there any fundamentally faster methods?
  - Alex Kaiser tried "sparse grid" schemes, but got disappointing results – better results were obtained using 2-D or 3-D versions of tanh-sinh.