High-Precision Arithmetic and Mathematical Physics

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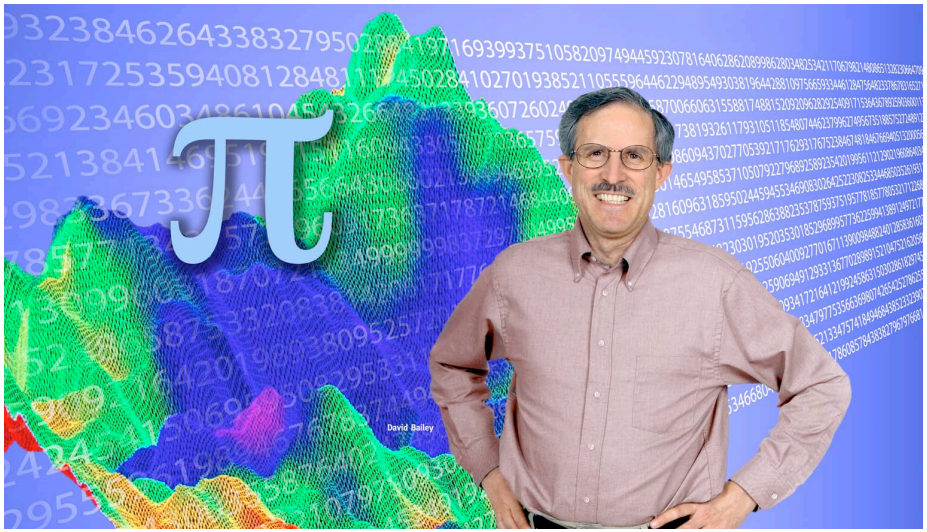


Online Resources for High-Precision Arithmetic and Experimental Math

- Experimental math website: http://www.experimentalmath.info
  Contains information and many links on experimental math.
- Inverse Symbolic Calculator, version 2: http://ddrive.cs.dal.ca/~isc/
  Online numeric constant recognition facility.
- LBNL's high-precision software: http://crd.lbl.gov/~dhbailey/mpdist
  Includes double-double, quad-double and arbitrary precision packages (C++ and Fortran-90). Also includes quadrature and PSLQ codes.
- Online experimental math toolkit: https://nebula.lbl.gov/cgi-bin/login.py
  Includes high-precision arithmetic, quadrature and PSLQ.
- *Mathematica* implementation of PSLQ:
  http://crd.lbl.gov/~dhbailey/mpdist/pslq-code.nb
- *Mathematica* solutions of exercises:
  http://crd.lbl.gov/~dhbailey/mpdist/sum-exercises.nb
  http://crd.lbl.gov/~dhbailey/mpdist/integral-exercises.nb

Applications of High-Precision Arithmetic in Modern Scientific Computing

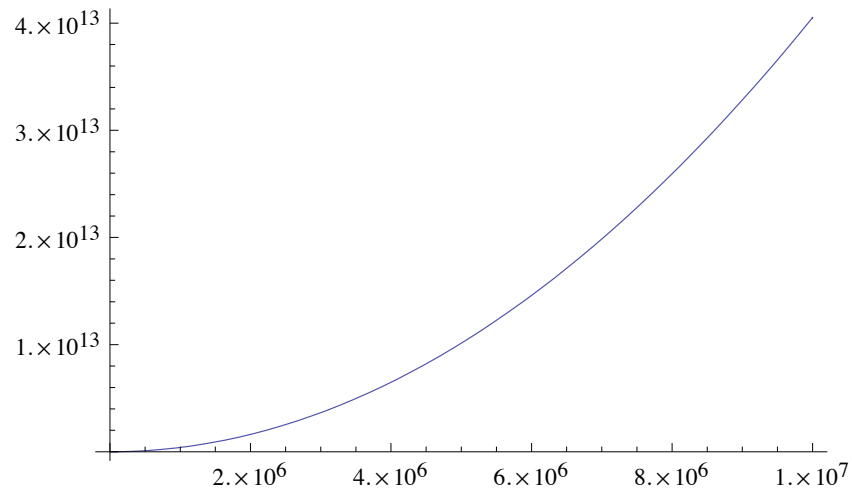
- Highly nonlinear computations.
- Computations involving highly ill-conditioned linear systems.
- Computations involving data with very large dynamic range.
- Large computations on highly parallel computer systems.
- Computations where numerical sensitivity is not currently a major problem, but periodic testing is needed to ensure that results are reliable.
- Research problems in mathematics and mathematical physics that involve constant recognition and integer relation detection.

Few physicists, chemists or engineers are highly expert in numerical analysis. Thus high-precision arithmetic is often a better remedy for severe numerical round-off error, even if the error could, in principle, be improved with more advanced algorithms or coding techniques.

Growth of Condition Number with System Size

Consider the very simple differential equation $y''(x) = -f(x)$. Discretization leads to the matrix:

$$\begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdots & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & -1 & 2 \end{bmatrix}$$



The condition number of this matrix (the quotient of the largest eigenvalue to the smallest eigenvalue) is readily seen to be approximately

$$\kappa(n) \approx \frac{4(n+1)^2}{\pi^2}$$

For modest-sized *n*, many systems of this type (depending on the right-hand side) cannot be reliably solved using 64-bit arithmetic.

Available High-Precision Facilities

Vendor-supported arithmetic:

Type	Total Bits	Significant Digits	Support
IEEE Double	64	16	In hardware on almost all systems.
IEEE Extended	80	18	In hardware on Intel and AMD systems.
IEEE Quad	128	33	In software from some vendors (50-100X slower than IEEE double).

Non-commercial (free) software:

Type	Total Bits	Significant Digits	Support
Double-double	128	32	DDFUN90, QD.
Quad-double	256	64	QD.
Arbitrary	Any	Any	ARPREC, MPFUN90, GMP, MPFR.

Commercial software: *Mathematica, Maple*.

LBNL's High-Precision Software

- QD: double-double (31 digits) and quad-double (62 digits).
- ARPREC: arbitrary precision.
- Low-level routines written in C++.
- C++ and Fortran-90 translation modules permit use with existing C++ and Fortran-90 programs -- only minor code changes are required.
- Includes many common functions: sqrt, cos, exp, gamma, etc.
- PSLQ, root finding, numerical integration.

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

Authors: Xiaoye Li, Yozo Hida, Brandon Thompson and DHB

GMP and MPFR

GNU Multiprecision Library:

- High-level signed integer arithmetic functions (mpz).
- High-level rational arithmetic functions (mpq).
- High-level floating-point arithmetic functions (mpf).
- C++ class-based interface to all of the above.

Available at: http://gmplib.org/

MPFR:

- C library of floating-point accurately rounding arithmetic functions.

Available at: http://www.mpfr.org

C++ high-level interfaces based on MPFR:

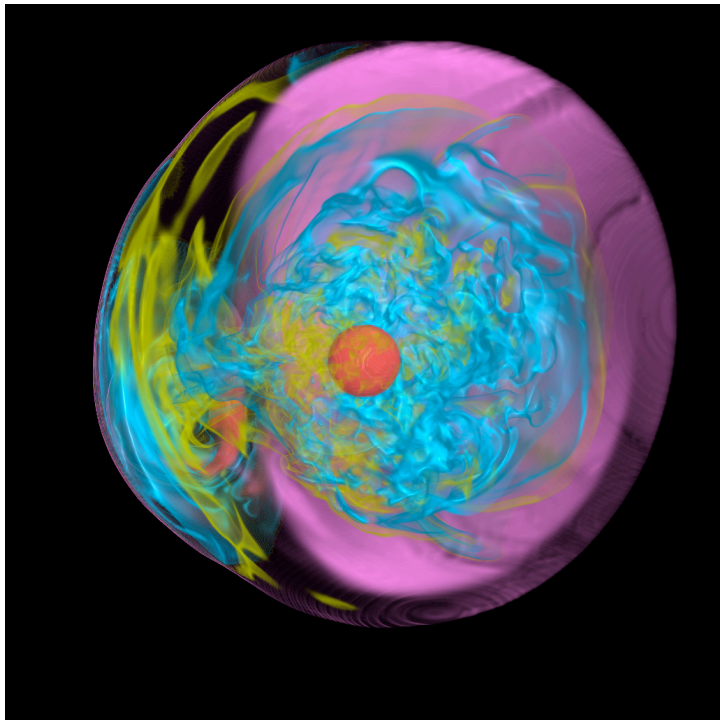
- MPFRCPP
- MPFR++
- GMPFRXX

Some Real-World Applications of High-Precision Arithmetic

- Supernova simulations (32 or 64 digits).
- Climate modeling (32 digits).
- Planetary orbit calculations (32 digits).
- Coulomb n-body atomic system simulations (32-120 digits).
- Schrodinger solutions for lithium and helium atoms (32 digits).
- Electromagnetic scattering theory (32-100 digits).
- Studies of the fine structure constant of physics (32 digits).
- Scattering amplitudes of quarks, gluons and bosons (32 digits).
- Theory of nonlinear oscillators (64 digits).

Application of High-Precision Arithmetic: Supernova Simulations

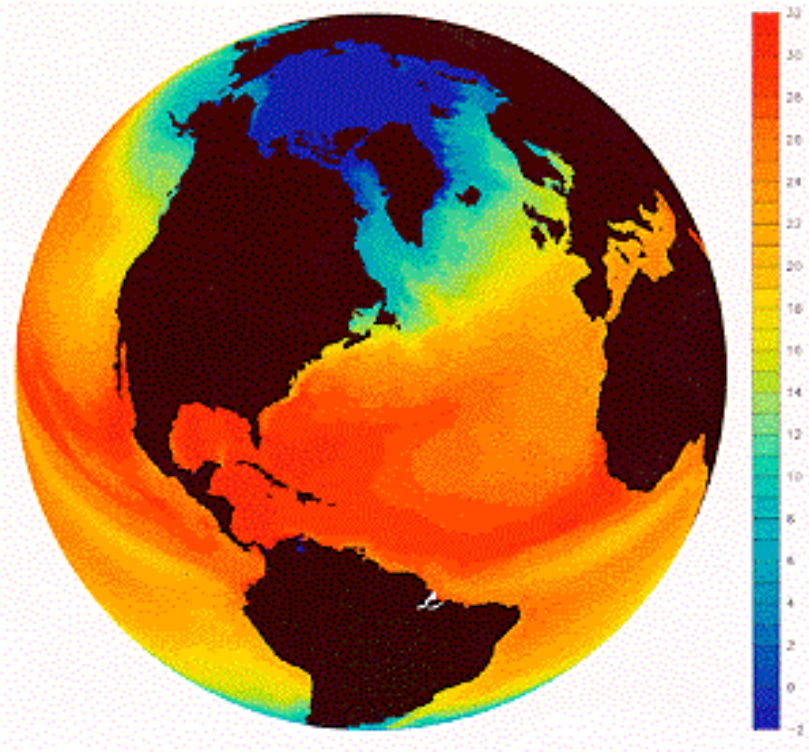
- Researchers at LBNL are using QD to solve for non-local thermodynamic equilibrium populations of iron and other atoms in the atmospheres of supernovas.
- Iron may exist in several species, so it is necessary to solve for all species simultaneously.
- Since the relative population of any state from the dominant state is proportional to the exponential of the ionization energy, the dynamic range of these values can be very large.
- The quad-double portion now dominates the entire computation.



P. H. Hauschildt and E. Baron, "The numerical solution of the expanding stellar atmosphere problem," *Journal Computational and Applied Mathematics*, vol. 109 (1999), pg. 41-63.

Climate Modeling

- Climate and weather simulations are fundamentally chaotic – if microscopic changes are made to the current state, soon the future state is quite different.
- In practice, computational results are altered even if minor changes are made to the code or the system.
- This numerical variation is a major nuisance for code maintenance.
- He and Ding of LBNL found that by using double-double arithmetic to implement a key inner product loop, most of this numerical variation disappeared.



Yun He and Chris Ding, "Using accurate arithmetics to improve numerical reproducibility and stability in parallel applications," *Journal of Supercomputing*, vol. 18, no. 3 (Mar 2001), pg. 259-277.

Planetary Orbit Calculations

- A key question of planetary theory is whether the solar system is stable over cosmological time frames (billions of years).
- Scientists have studied this question by performing very long-term simulations of planetary motions.
- This problem is well known to exhibit chaos.
- Simulations typically do well for long periods of time, but then fail at certain key junctures, unless special measures are taken.
- Researchers have found that double-double or quad-double arithmetic is required to avoid severe numerical inaccuracies, even if other techniques are employed.

"The orbit of any one planet depends on the combined motions of all the planets, not to mention the actions of all these on each other. To consider simultaneously all these causes of motion and to define these motions by exact laws allowing of convenient calculation exceeds, unless I am mistaken, the forces of the entire human intellect." [Isaac Newton, 1687]

G. Lake, T. Quinn and D. C. Richardson, "From Sir Isaac to the Sloan survey: Calculating the structure and chaos due to gravity in the universe," *Proceedings of the Eighth Annual ACM-SIAM Symposium on Discrete Algorithms*, SIAM, Philadelphia, 1997, pg. 1-10.

Coulomb N-Body Atomic System Simulations

- Alexei Frolov of Queen's University in Canada has used MPFUN90 to solve a generalized eigenvalue problem that arises in Coulomb n-body interactions.
- Matrices are typically 5,000 x 5,000 and are very nearly singular.
- Frolov has also computed elements of the Hamiltonian matrix and the overlap matrix in four- and five-body systems.
- These computations typically require 120-digit arithmetic.

"We can consider and solve the bound state few-body problems which have been beyond our imagination even four years ago." – Frolov

A. M. Frolov and DHB, "Highly accurate evaluation of the few-body auxiliary functions and four-body integrals," *Journal of Physics B*, vol. 36, no. 9 (14 May 2003), pg. 1857-1867.

High-Precision Arithmetic and Experimental Mathematics

"Experimental" methodology:

- Compute various mathematical entities (limits, infinite series sums, definite integrals) to high precision.
- Use algorithms such as PSLQ to recognize these entities in terms of well-known mathematical constants.
- Use this same process to discover relations between entities.
- When results are found experimentally, seek to find formal mathematical proofs of the discovered relations.
- Many results have been found using this methodology, both in pure math and in mathematical physics.

1. J. M. Borwein and DHB, *Mathematics by Experiment: Plausible Reasoning in the 21st Century*, A.K. Peters, 2004. Second edition 2008.
2. J. M. Borwein, DHB and R. Girgensohn, *Experimentation in Mathematics: Computational Paths to Discovery*, A.K. Peters, 2004.
3. DHB, J. M. Borwein, N. J. Calkin, R. Girgensohn, D. R. Luke, V. Moll, *Experimental Mathematics in Action*, A.K. Peters, 2007.
4. J. M. Borwein and K. Devlin, *The Computer as Crucible: An Introduction to Experimental Mathematics*, A.K. Peters, 2007.

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).

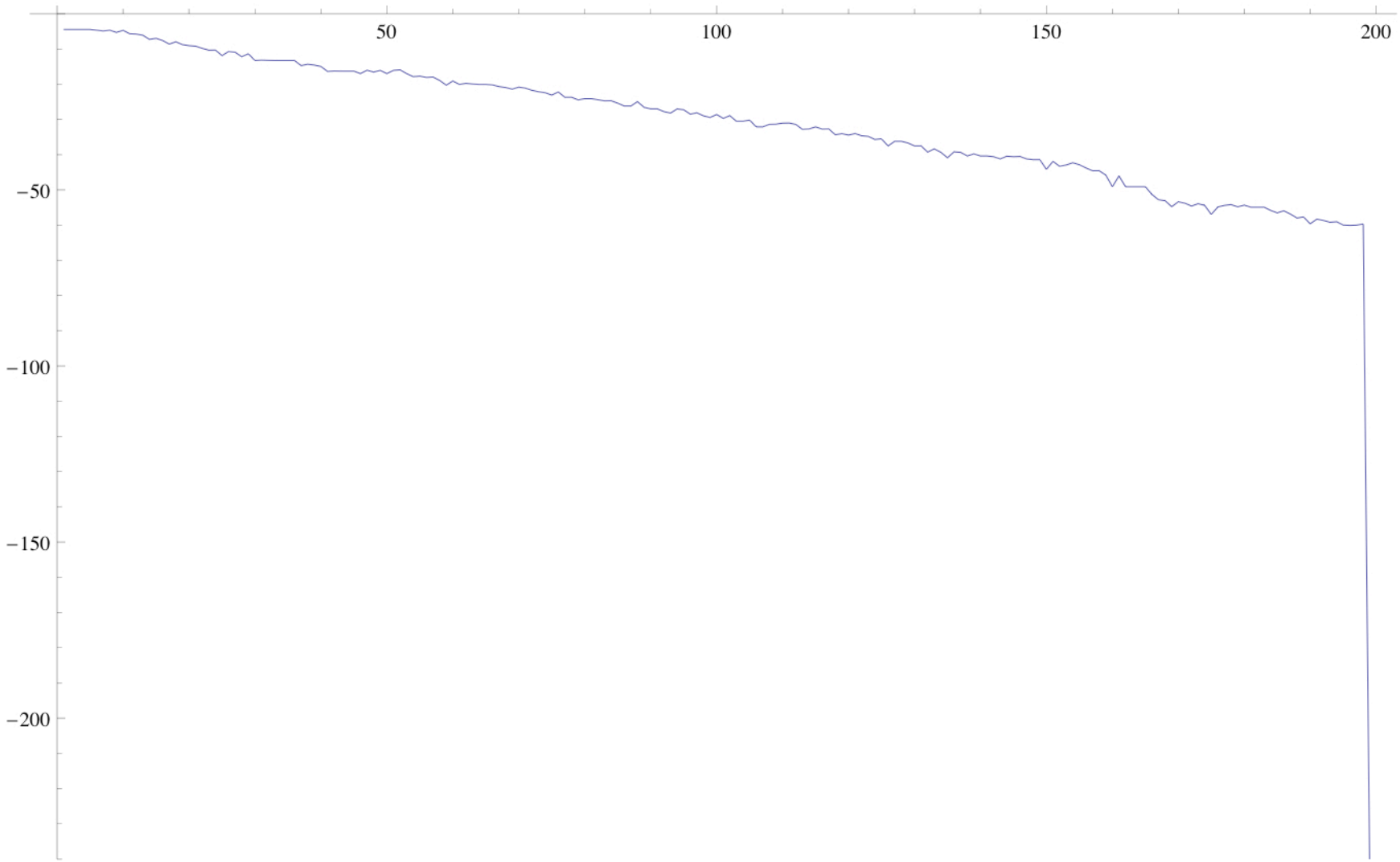
At the present time the "PSLQ" algorithm of mathematician-sculptor Helaman Ferguson is the most widely used integer relation algorithm. It was named one of ten "algorithms of the century" by *Computing in Science and Engineering*.

1. H. R. P. Ferguson, DHB and S. Arno, "Analysis of PSLQ, an integer relation finding algorithm," *Mathematics of Computation*, vol. 68, no. 225 (Jan 1999), pg. 351-369.
2. DHB and D. J. Broadhurst, "Parallel integer relation detection: Techniques and applications," *Mathematics of Computation*, vol. 70, no. 236 (Oct 2000), pg. 1719-1736.

PSLQ, Continued

- PSLQ constructs a sequence of integer-valued matrices B_n that reduces the vector $y = x\,B_n$, until either the relation is found (as one of the columns of B_n), or else precision is exhausted.
- At the same time, PSLQ generates a steadily growing bound on the size of any possible relation.
- 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).
- 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.
- PSLQ (or any other integer relation scheme) requires *very high precision arithmetic* (at least nd 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.

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

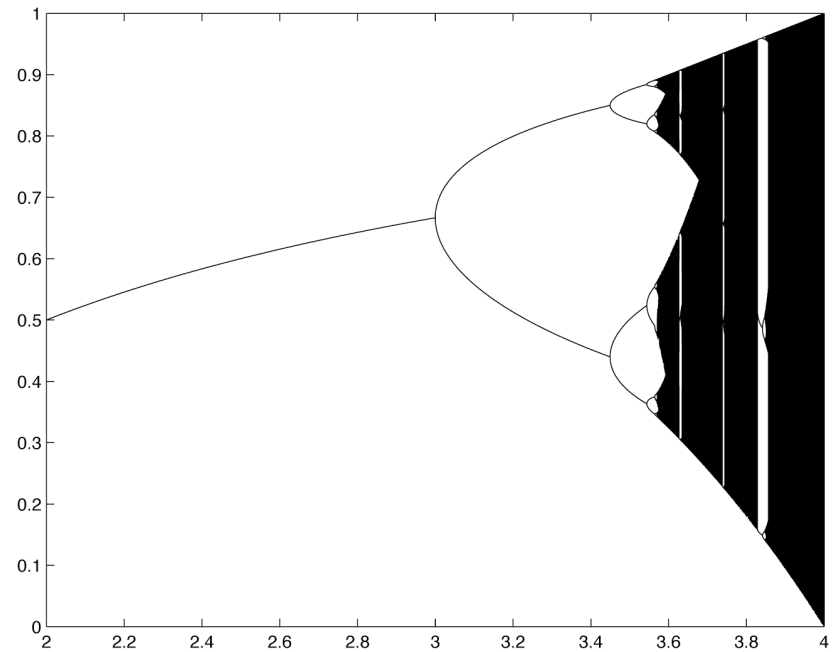
- Calculate α to high precision – typically 100 - 1000 digits. This is often the most computationally expensive part of the entire process.
- Based on experience with similar constants or relations, make a list of possible terms on the right-hand side (RHS) of a linear formula for α, then calculate each of the *n* RHS terms to the same precision as α.
- If you suspect α is algebraic of degree *n* (the root of a degree-*n* polynomial with integer coefficients), compute the vector $(1, \alpha, \alpha^2, \alpha^3, \ldots, \alpha^n)$.
- Apply PSLQ to the $(n+1)$-long vector, using the same numeric precision as α, but with a detection threshold a few orders of magnitude larger than "epsilon"– e.g., 10^{-480} instead of 10^{-500} for 500-digit arithmetic.
- When PSLQ runs, look for a detection following a drop in the size of the reduced *y* vector by at least 20 orders of magnitude, to value near epsilon.
- If no credible relation is found, try expanding the list of RHS terms.
- Another possibility is to search for multiplicative relations (i.e., monomial expressions), which can be done by taking logarithms of α and constants.

Bifurcation Points in Chaos Theory

Let $t = B_3$ = the smallest r such that the "logistic iteration"

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

exhibits 8-way periodicity instead of 4-way periodicity.



By means of a sequential approximation scheme, one can obtain the numerical value of t to any desired precision:

3.544090359551922853615965986604804540583099845444573675457812
5303058429428588630122562585664248917999626…

Applying PSLQ to (1, t, t^2, t^3, …, t^{12}), we obtained the result that t is a root of:

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

PSLQ and Sculpture

The complement of the figure-eight knot (see Ferguson's sculpture at right) when viewed in hyperbolic space, has volume

V = 2.029883212819307250042…

Recently British physicist David Broadhurst found (using PSLQ) that

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

and thus *V*/sqrt(3) is a base-3 BBP-type constant (see next section).

J. M. Borwein and D. H. Bailey, *Mathematics by Experiment*, A.K. Peters, 2004, pg. 53.

The Borwein-Plouffe Observation

In 1996, Peter Borwein and Simon Plouffe observed that the following well-known formula for $\log_e(2)$

$$\log 2 = \sum_{n=1}^{\infty} \frac{1}{n 2^n} = 0.693147180559945309417232121458\ldots$$

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

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

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

Fast Exponentiation Mod *n*

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:

Simple example problem: Calculate the 3^{17} mod 10.

Algorithm A: 3x3x3x3x3x3x3x3x3x3x3x3x3x3x3x3x3 = 129140163. Ans =3.

Algorithm B: $3^{17} = (((3^2)^2)^2)^2 \times 3 = 129140163$. Ans = 3.

Algorithm C:

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

In detail: $3^2 \bmod 10 = 9$; $9^2 \bmod 10 = 1$; $1^2 \bmod 10 = 1$; $1^2 \bmod 10 = 1$; $1 \times 3 = 3$. Ans = 3. You can do this "in your head"!

Note that with Algorithm C, we never have to deal with integers > 81 = $(n-1)^2$. For large n, this is a huge computational savings.

The BBP Formula for Pi

In 1996, at the suggestion of Peter Borwein, Simon Plouffe used DHB's PSLQ program and arbitrary precision software to discover this new formula for π:

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

This formula permits one to compute binary (or hexadecimal) digits of π beginning at an arbitrary starting position, using a very simple scheme that can run on any system with standard 64-bit or 128-bit arithmetic.

Recently it was proven that no base-*n* formulas of this type exist for π, except $n = 2^m$.

1. DHB, 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 New BBP-Type Formulas Discovered Using PSLQ

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

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

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

DHB, “A compendium of BBP-type formulas,” at http://crd.lbl.gov/~dhbailey/dhbpapers/bbp-formulas.pdf.

Computing High-Precision Limits of Sequences

The most commonly used scheme to compute a high-precision limit of a sequence (x_n) is Richardson's extrapolation: Define $A_{1,1} = x_1$. Then iteratively set $A_{n,1} = x_n$, at the same time using this recursion for $k = 2$ to n to generate the n-th row of the lower-triangular matrix A:

$$A_{n,k} = \frac{2^k A_{n,k-1} - A_{n-1,k-1}}{2^k - 1}$$

Then the successive diagonal entries $A_{n,n}$ are increasingly accurate estimates for the limiting value.

Avram Sidi, *Practical Extrapolation Methods: Theory and Applications*, Cambridge University Press, 2002, pg. 21-41.

The Quinn-Rand-Strogatz Constant of Nonlinear Physics

Quinn, Rand, and Strogatz recently described a nonlinear oscillator system by means of the formula

$$0 = \sum_{i=1}^{N} \left(2\sqrt{1 - s^2(1 - 2(i-1)/(N-1))^2} - \frac{1}{\sqrt{1 - s^2(1 - 2(i-1)/(N-1))^2}} \right)$$

For large *N*, *s* = 1 – *c* / *N* (approx), where *c* = 0.6054436... Strogatz asked us to validate and extend this computation, and challenged us to identify this limit if it exists.

By means of a Richardson extrapolation scheme, implemented on 64-CPUs of a highly parallel computer system, we computed (using the QD software)

c = 0.605443657196732749478922842447207475220899 6…

This led to the provable conclusion that the limit *c* exists and is the root of a Hurwitz zeta function (below). As a bonus, we obtained some asymptotic terms.

$$\zeta(1/2, x/2) = 0$$

DHB, J.M, Borwein and R.E. Crandall, “Resolution of the Quinn-Rand-Strogatz constant of nonlinear physics,” *Experimental Mathematics*, vol. 18 (2009), pg. 107-116.

Euler's Technique for Accelerating Sums of Alternating Infinite Series

$$
\begin{aligned}
\sum_{k=0}^{\infty}(-1)^k u_k &= \sum_{m=0}^{n-1}(-1)^k u_k + \sum_{k=0}^{\infty}\frac{(-1)^k \Delta^k u_n}{2^{k+1}} \\
\Delta^1 u_n &= u_{n+1} - u_n \\
\Delta^2 u_n &= \Delta^1 u_{n+1} - \Delta^1 u_n \;=\; u_{n+2} - 2u_{n+1} + u_n \\
\Delta^3 u_n &= \Delta^2 u_{n+2} - \Delta^2 u_{n+1} \;=\; u_{n+3} - 3u_{n+2} + 3u_{n+1} - u_n \\
&\ldots
\end{aligned}
$$

For example, Catalan's constant = $1 - 1/3^2 + 1/5^2 - 1/7^2 + 1/9^2 \ldots$ can be computed to 500-digit precision by setting n = 1000, then evaluating 400 terms of the second series (a total of 1400 function evaluations).

William H. Press, et al, *Numerical Recipes*, Cambridge University Press, 1966, pg. 133-134.

Converting All-Positive Series to Alternating Series

Given an all-positive series (x_n), one can construct an alternating series (y_n) with the same sum as follows: Set $y_0 = x_0$, then for $n > 0$

$$y_n = (-1)^n \sum_{k=0}^{\infty} 2^k x_{n2^k}$$

Each of these individual summations converges quite rapidly, so only a modest number of terms typically need to be computed. Euler's technique can then be applied to find the sum

$$S = \sum_{n=0}^{\infty} y_n = \sum_{n=0}^{\infty} x_n$$

This method works fairly well, but is many times more costly than the alternating series case. Is there an efficient, general-purpose, numerically robust scheme for finding high-precision values for infinite series sums?

Multivariate Zeta Sums

In April 1993, Enrico Au-Yeung, an undergraduate at the University of Waterloo, brought to the attention of Jonathan Borwein the claim (based on numerical calculation) that

$$\sum_{k=1}^{\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^2 k^{-2} \quad = \quad \frac{17\pi^4}{360}$$

Borwein was very skeptical, but subsequent computations affirmed this to high precision, and the result was proved. Many other similar identities were subsequently discovered. This sum is a special case of the following class:

$$\zeta(s_1, s_2, \cdots, s_k) \quad = \quad \sum_{n_1>n_2>\cdots n_k>0} \prod_{j=1}^{k} n_j^{-s_j}\sigma_j^{-n_j}$$

where s_j are integers and σ_j = sign of s_j. These can be rapidly computed using the Euler summation technique, or with the online tool at http://www.cecm.sfu.ca/projects/ezface+.

1. J. M. Borwein and DHB, *Mathematics by Experiment*, A.K. Peters, 2004 (2nd ed. 2008), pg. 56.

2. J. M. Borwein, DHB and Roland Girgensohn, *Experimentation in Mathematics*, A.K. Peters, 2004, pg 142-160.

Multivariate Zeta Example

Consider this example:

$$s_{2,3} = \sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \cdots + \frac{(-1)^{k+1}}{k}\right)^2 (k+1)^{-3}$$

Using numerical methods (Euler or EZFACE+) , one obtains this value:

0.156166933381176915881035909687988193685776709840303872957529354497075037440295791455205653709358147578...

Using PSLQ, we found this evaluation:

$$s_{2,3} = 4\mathrm{Li}_5\left(\frac{1}{2}\right) - \frac{1}{30}\log^5(2) - \frac{17}{32}\zeta(5) - \frac{11}{720}\pi^4\log(2) + \frac{7}{4}\zeta(3)\log^2(2) + \frac{1}{18}\pi^2\log^3(2) - \frac{1}{8}\pi^2\zeta(3)$$

Here $\mathrm{Li}_n(x) = x^k k^{-n}$ is the polylogarithm function and $\zeta(x)$ is the Riemann zeta function.

History of Numerical Integration (Quadrature)

- 1670: Newton devises the Newton-Coates integration rule.
- 1740: Thomas Simpson develops Simpson's rule.
- 1820: Gauss develops Gaussian quadrature.
- 1950-1970: Adaptive quadrature, Romberg integration, Clenshaw-Curtis integration, others.
- 1973: Takashi and Mori develop the tanh-sinh quadrature scheme.
- 1985-1990: Maple and Mathematica feature built-in numerical quadrature facilities.
- 2000: Very high-precision quadrature (1000+ digits) methods.

With high-precision numerical values, we can now use PSLQ to obtain analytical evaluations of integrals.

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 $\cos[\pi(j\text{-}1/4)/(n\text{+}1/2)]$. Legendre polynomials and their derivatives can be computed using the formulas $P_0(x) = 0$, $P_1(x) = 1$,

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

DHB, 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

$$\int_a^b f(x)\,\mathrm{d}x = h\sum_{j=0}^{n} f(x_j) - \frac{h}{2}(f(a)+f(b))$$

$$-\sum_{i=1}^{m} \frac{h^{2i}B_{2i}}{(2i)!}\left(D^{2i-1}f(b) - D^{2i-1}f(a)\right) - E(h)$$

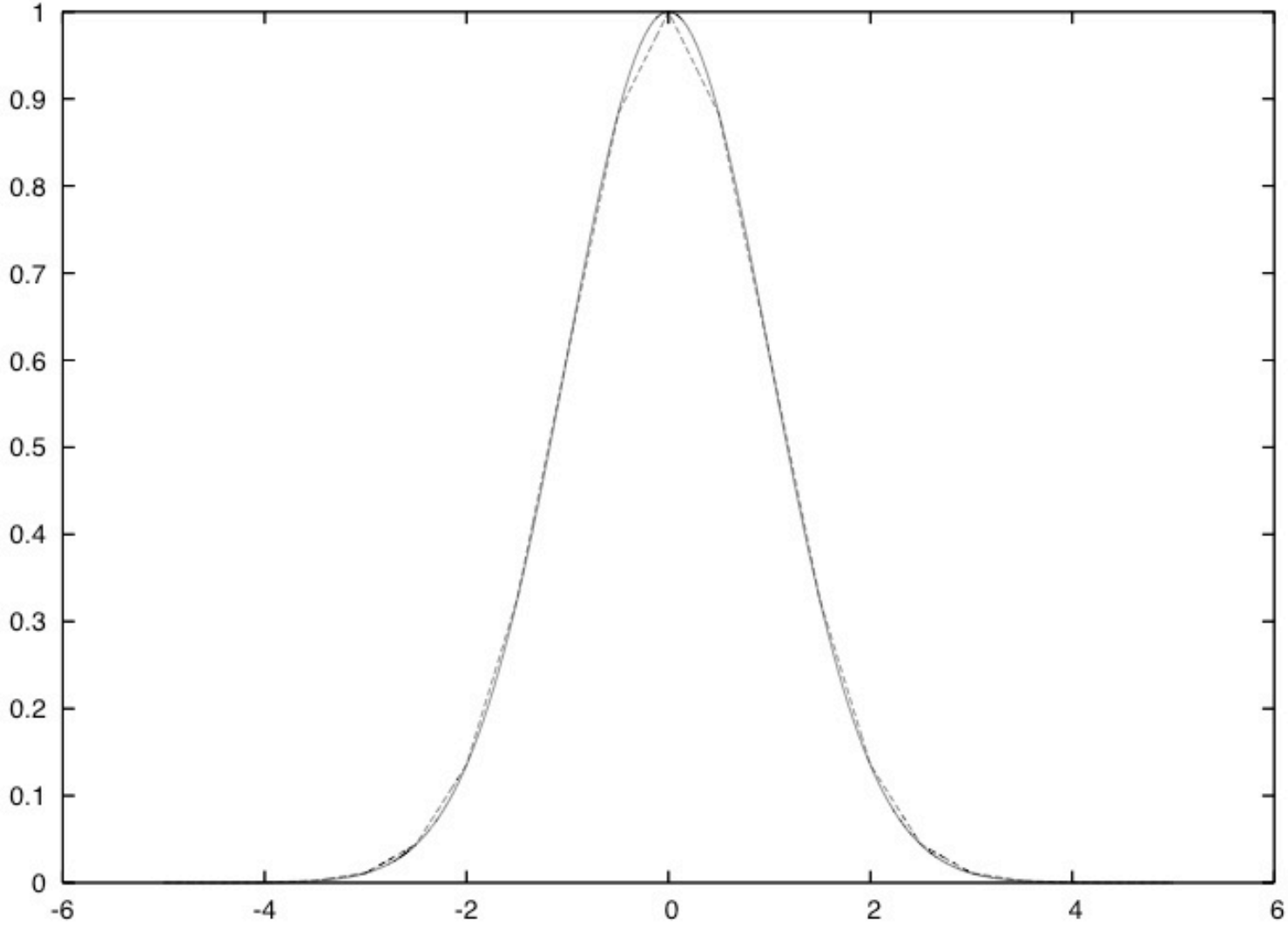
$$|E(h)| \leq 2(b-1)(h/(2\pi))^{2m+2} \max_{a\leq x\leq b} |D^{2m+2}f(x)|$$

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 $f(x)$.

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 (π/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 $w_j = g'(hj)$. 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 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.

In our experience, 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 its computation of abscissas and weights is much faster than other schemes.

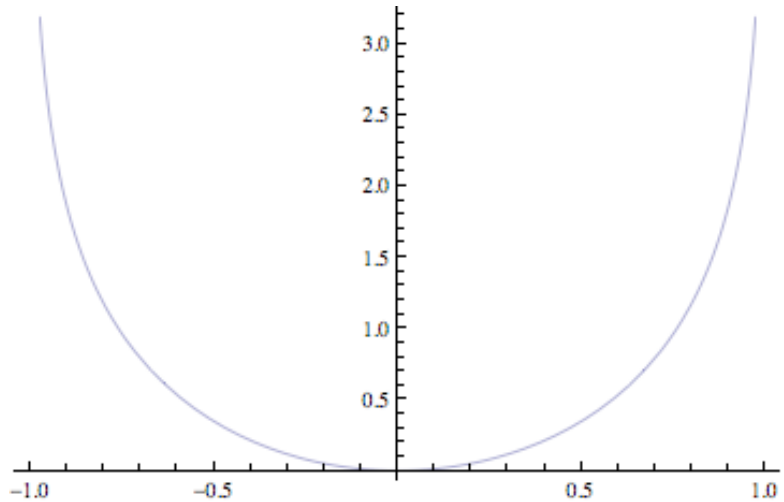
1. DHB, X.S. Li and K. Jeyabalan, "A comparison of three high-precision quadrature schemes," *Experimental Mathematics*, vol. 14 (2005), no. 3, pg. 317-329.
2. H. Takahasi and M. Mori, "Double exponential formulas for numerical integration," Publications of RIMS, Kyoto University, vol. 9 (1974), pg.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

Original and Transformed Integrand Functions

Original integrand function on [-1,1]:

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

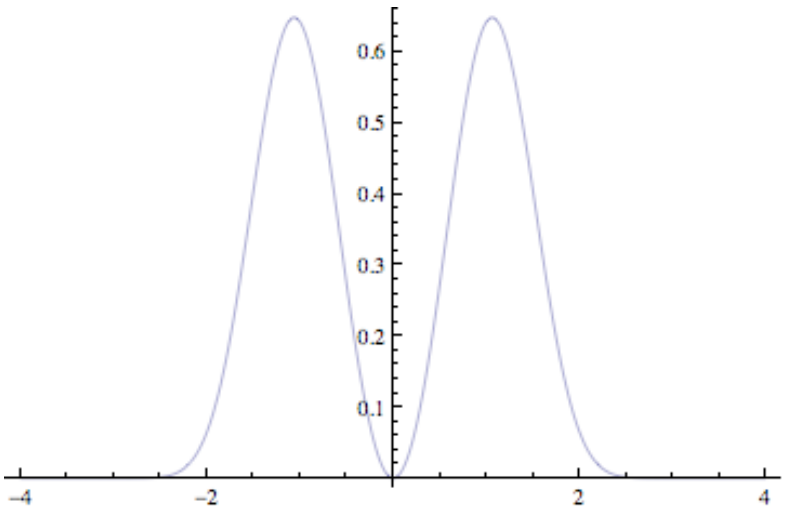
Note the singularities at the endpoints.



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

$$f(g(t))g'(t) \quad = \quad -\log\cos[\pi/2 \cdot \tanh(\sinh t)]\left(\frac{\cosh(t)}{\cosh(\sinh t)^2}\right)$$

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



Quadrature and PSLQ: Example 1

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

For various arguments, quadrature followed by PSLQ yields results such as

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

Here *G* is Catalan's constant. Several general results have now been proven, including

$$\int_0^\infty \frac{\arctan\sqrt{x^2+a^2}}{(x^2+1)\sqrt{x^2+a^2}}\,\mathrm{d}x = \frac{\pi}{2\sqrt{a^2-1}}\left(2\arctan\sqrt{a^2-1} - \arctan\sqrt{a^4-1}\right)$$

Quadrature and PSLQ: Example 2

$$\frac{2}{\sqrt{3}}\int_0^1 \frac{\log^6(x)\arctan(x\sqrt{3}/(x-2))}{x+1}\,\mathrm{d}x \quad =$$

$$\frac{1}{81648}\left(-229635L_3(8)+29852550L_3(7)\log 3-1632960L_3(6)\pi^2\right.$$
$$+27760320L_3(5)\zeta(3)-275184L_3(4)\pi^4+36288000L_3(3)\zeta(5)$$
$$\left.-30008L_3(2)\pi^6-57030120L_3(1)\zeta(7)\right)$$

where

$$L_{-3}(s)=\sum_{n=1}^{\infty}\left(\frac{1}{(3n-2)^s}-\frac{1}{(3n-1)^s}\right)$$

is the Dirichlet series. Numerous other related results have been found.

D. H. Bailey, et. al, *Experimental Mathematics in Action*, A.K. Peters, 2007, pg. 43,44,61.

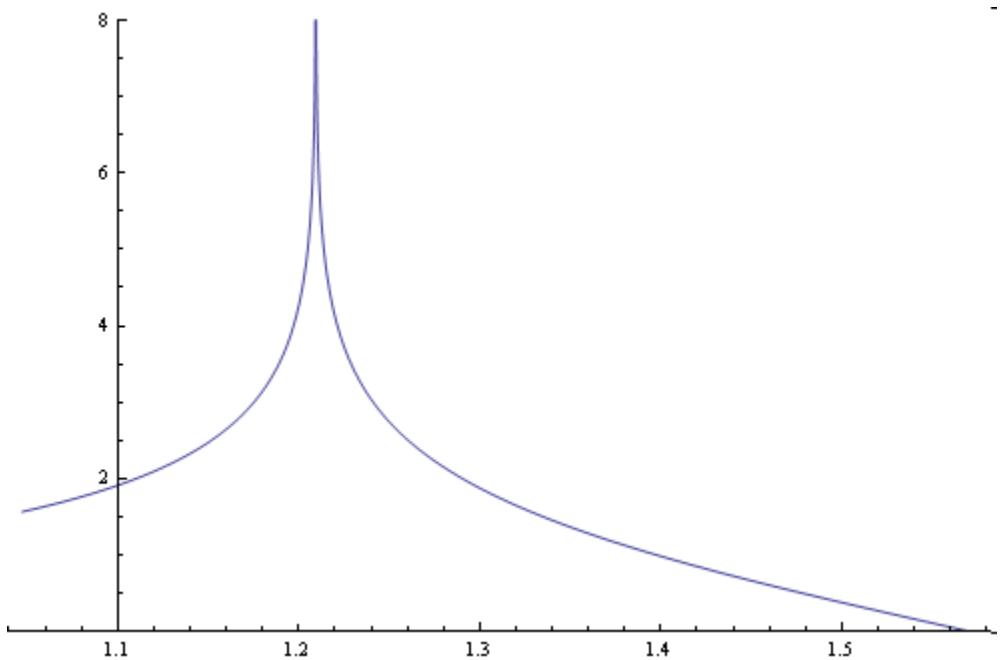
A Log-Tan Integral Identity

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

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

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 highly parallel tanh-sinh quadrature). A proof is now known.



DHB, 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 .

Integrals on Semi-Infinite Intervals

When using either by Gaussian quadrature or tanh-sinh quadrature, integrals on (0,infinity) can be computed by making the simple substitution $s = 1/t$:

$$\int_0^\infty f(t)\,\mathrm{d}t = \int_0^1 f(t)\,\mathrm{d}t + \int_1^\infty f(t)\,\mathrm{d}t = \int_0^1 f(t)\,\mathrm{d}t + \int_0^1 f(1/s)/s^2\,\mathrm{d}s$$

Integrals of oscillating functions on a semi-infinite interval can be computed accurately by the following scheme: let $x = g(t) = M\,t\,/\,(1 - \exp(-2\,\pi \sinh t))$, so that, for instance, the integral of $\mathrm{sinc}(x) = \sin(x)/x$ on (0,infinity) becomes:

$$\begin{aligned}\int_0^\infty \sin(x)/x\,\mathrm{d}x &= \int_{-\infty}^\infty \sin(g(t))/g(t)\cdot g'(t)\,\mathrm{d}t \\ &\approx h\sum_{k=-\infty}^{\infty} \sin(g(hk))/g(hk)\cdot g'(hk)\end{aligned}$$

If one chooses $M = \pi/h$, then note that for large k, the $g(h\,k)$ values are all very close to $k\,\pi$, so the $\sin(g(hk))$ values are all very close to zero. Thus the sum can be truncated after a moderate number of terms, as in tanh-sinh.

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.

Computing High-Precision Values of Multi-Dimension Integrals

Computing multi-hundred digit numerical values of 2-D, 3-D and higher-dimensional integrals remains a major challenge.

Typical approach:

- Consider the 2-D or 3-D domain divided into 1-D lines.
- Use Gaussian quadrature (for regular functions) or tanh-sinh quadrature (if function has vertical derivates or singularities on boundaries) on each of the 1-D lines.
- Discontinue evaluation beyond points where it is clear that function-weight products are smaller than the “epsilon” of the precision level (this works better with tanh-sinh).

Even with “smart” evaluation that avoids unnecessary evaluations, the computational cost increases very sharply with dimension:

- If 1000 evaluation points are required in 1-D for a given precision, then typically 1,000,000 are required in 2-D and 1,000,000,000 in 3-D, etc.

The Sparse Grid Scheme

The "sparse grid" scheme for numerical integration in multiple dimensions approximates an integral by evaluating a succession of nested lower-resolution quadrature rules. For example, in two dimensions:

- Level 1: 1x1 (i.e., evaluate function only at origin)
- Level 2: (1x3 + 3x1) – (1x1)
- Level 3: (1x5 + 3x3 + 5x1) – (1x3 + 3x1)
- Level 4: (1x9 + 3x5 + 5x3 + 9x1) – (1x5 + 3x3 + 5x1)
- Level 5: (1x17 + 3x9 + 5x5 + 9x3 + 17x1) – (1x9 + 3x5 + 5x3 + 9x1)

The sparse grid theory shows that for broad classes of functions, this multi-level scheme achieves reasonably fast convergence.

Note that in high dimensions, most points are a relatively far distance from the origin, where the multi-dimensional weight of the quadrature scheme (and, most likely, the function itself) have small values.

Thus a nested scheme (like sparse grid) that avoids the distant "corners" achieves a significant savings in high dimensions.

Ising Integrals

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 $u_k = t_1\, t_2 \ldots t_k$.

DHB, 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:

$$C_1 = 2$$

$$C_2 = 1$$

$$C_3 = \mathrm{L}_{-3}(2) = \sum_{n \geq 0} \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right)$$

$$C_4 = \frac{7}{12} \zeta(3)$$

Limiting Value of C_n

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://ddrive.cs.dal.ca/~isc

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

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

where $\mathrm{Li}_n(x)$ 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 an 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 \Big[2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 \\
& \Big(-\big[4(x+1)(xy+1)\log(2)\left(y^5z^3x^7-y^4z^2(4(y+1)z+3)x^6-y^3z\left(\left(y^2+1\right)z^2+4(y+1)z+5\right)x^5+y^2\left(4y(y+1)z^3+3\left(y^2+1\right)z^2+4(y+1)z-1\right)x^4+y\left(z\left(z^2+4z+5\right)y^2+4\left(z^2+1\right)y+5z+4\right)x^3+\left(\left(-3z^2-4z+1\right)y^2-4zy+1\right)x^2-(y(5z+4)+4)x-1\right)\big]\big/\left[(x-1)^3(xy-1)^3(xyz-1)^3\right]+\big[3(y-1)^2y^4(z-1)^2z^2(yz-1)^2x^6+2y^3z\left(3(z-1)^2z^3y^5+z^2\left(5z^3+3z^2+3z+5\right)y^4+(z-1)^2z\left(5z^2+16z+5\right)y^3+\left(3z^5+3z^4-22z^3-22z^2+3z+3\right)y^2+3\left(-2z^4+z^3+2z^2+z-2\right)y+3z^3+5z^2+5z+3\right)x^5+y^2\left(7(z-1)^2z^4y^6-2z^3\left(z^3+15z^2+15z+1\right)y^5+2z^2\left(-21z^4+6z^3+14z^2+6z-21\right)y^4-2z\left(z^5-6z^4-27z^3-27z^2-6z+1\right)y^3+\left(7z^6-30z^5+28z^4+54z^3+28z^2-30z+7\right)y^2-2\left(7z^5+15z^4-6z^3-6z^2+15z+7\right)y+7z^4-2z^3-42z^2-2z+7\right)x^4-2y\left(z^3\left(z^3-9z^2-9z+1\right)y^6+z^2\left(7z^4-14z^3-18z^2-14z+7\right)y^5+z\left(7z^5+14z^4+3z^3+3z^2+14z+7\right)y^4+\left(z^6-14z^5+3z^4+84z^3+3z^2-14z+1\right)y^3-3\left(3z^5+6z^4-z^3-z^2+6z+3\right)y^2-\left(9z^4+14z^3-14z^2+14z+9\right)y+z^3+7z^2+7z+1\right)x^3+\left(z^2\left(11z^4+6z^3-66z^2+6z+11\right)y^6+2z\left(5z^5+13z^4-2z^3-2z^2+13z+5\right)y^5+\left(11z^6+26z^5+44z^4-66z^3+44z^2+26z+11\right)y^4+\left(6z^5-4z^4-66z^3-66z^2-4z+6\right)y^3-2\left(33z^4+2z^3-22z^2+2z+33\right)y^2+\left(6z^3+26z^2+26z+6\right)y+11z^2+10z+11\right)x^2-2\left(z^2\left(5z^3+3z^2+3z+5\right)y^5+z\left(22z^4+5z^3-22z^2+5z+22\right)y^4+\left(5z^5+5z^4-26z^3-26z^2+5z+5\right)y^3+\left(3z^4-22z^3-26z^2-22z+3\right)y^2+\left(3z^3+5z^2+5z+3\right)y+5z^2+22z+5\right)x+15z^2+2z+2y(z-1)^2(z+1)+2y^3(z-1)^2z(z+1)+y^4z^2\left(15z^2+2z+15\right)+y^2\left(15z^4-2z^3-90z^2-2z+15\right)+15\big]\big/\left[(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2(xyz-1)^2\right]-\big[4(x+1)(y+1)(yz+1)\left(-z^2y^4+4z(z+1)y^3+\left(z^2+1\right)y^2-4(z+1)y+4x\left(y^2-1\right)\left(y^2z^2-1\right)+x^2\left(z^2y^4-4z(z+1)y^3-\left(z^2+1\right)y^2+4(z+1)y+1\right)-1\right)\log(x+1)\big]\big/\left[(x-1)^3x(y-1)^3(yz-1)^3\right]-\big[4(y+1)(xy+1)(z+1)\left(x^2\left(z^2-4z-1\right)y^4+4x(x+1)\left(z^2-1\right)y^3-\left(x^2+1\right)\left(z^2-4z-1\right)y^2-4(x+1)\left(z^2-1\right)y+z^2-4z-1\right)\log(xy+1)\big]\big/\left[x(y-1)^3y(xy-1)^3(z-1)^3\right]-\big[4(z+1)(yz+1)\left(x^3y^5z^7+x^2y^4(4x(y+1)+5)z^6-xy^3\left(\left(y^2+1\right)x^2-4(y+1)x-3\right)z^5-y^2\left(4y(y+1)x^3+5\left(y^2+1\right)x^2+4(y+1)x+1\right)z^4+y\left(y^2x^3-4y(y+1)x^2-3\left(y^2+1\right)x-4(y+1)\right)z^3+\left(5x^2y^2+y^2+4x(y+1)y+1\right)z^2+\left((3x+4)y+4\right)z-1\right)\log(xyz+1)\big]\big/\left[xy(z-1)^3z(yz-1)^3(xyz-1)^3\right]\Big)\Big] \\
& \big/\left[(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2\right]\;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*.

DHB, 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

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

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

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

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

DHB, 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

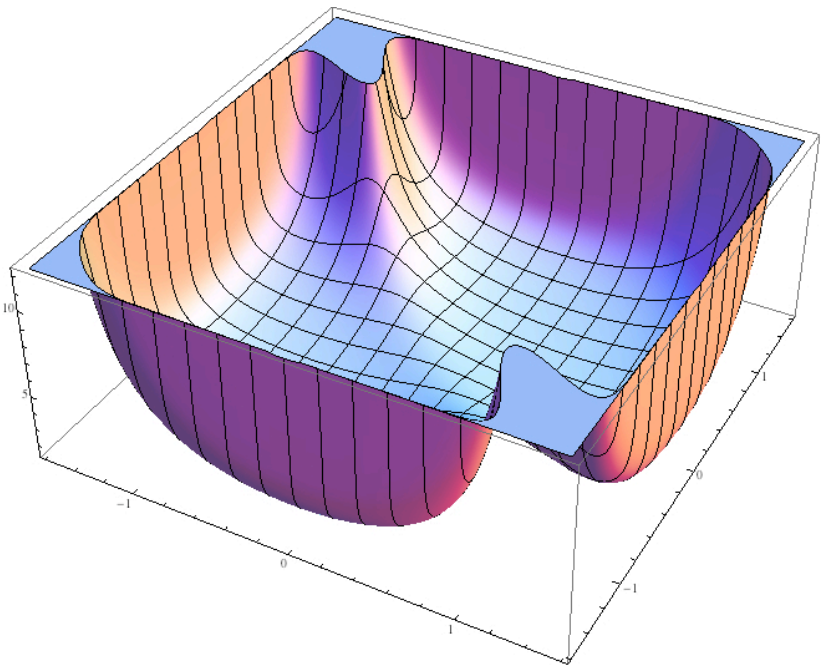
We conjectured (and later proved)

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

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.



Heisenberg Spin Integrals

In another recent application of these methods, we investigated the following "spin integrals," which arise from studies in mathematical physics:

$$P(n) \quad := \quad \frac{\pi^{n(n+1)/2}}{(2\pi i)^n} \cdot \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} U(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2)$$
$$\times\, T(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2)\, \mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_n$$

where

$$U(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) \;=\; \frac{\prod_{1 \le k < j \le n} \sinh[\pi(x_j - x_k)]}{\prod_{1 \le j \le n} i^n \cosh^n(\pi x_j)}$$

$$T(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) \;=\; \frac{\prod_{1 \le j \le n} (x_j - i/2)^{j-1} (x_j + i/2)^{n-j}}{\prod_{1 \le k < j \le n} (x_j - x_k - i)}$$

H. E. Boos, V. E. Korepin, Y. Nishiyama and M. Shiroishi, "Quantum correlations and number theory," *Journal of Physics A: Mathematical and General*, vol. 35 (2002), pg. 4443.

Evaluations of *P*(*n*) Derived Analytically, Confirmed Numerically

$$
\begin{aligned}
P(1) &= \frac{1}{2}, \quad P(2) = \frac{1}{3} - \frac{1}{3}\log 2, \quad P(3) = \frac{1}{4} - \log 2 + \frac{3}{8}\zeta(3) \\
P(4) &= \frac{1}{5} - 2\log 2 + \frac{173}{60}\zeta(3) - \frac{11}{6}\zeta(3)\log 2 - \frac{51}{80}\zeta^2(3) - \frac{55}{24}\zeta(5) + \frac{85}{24}\zeta(5)\log 2 \\
P(5) &= \frac{1}{6} - \frac{10}{3}\log 2 + \frac{281}{24}\zeta(3) - \frac{45}{2}\zeta(3)\log 2 - \frac{489}{16}\zeta^2(3) - \frac{6775}{192}\zeta(5) \\
&\quad + \frac{1225}{6}\zeta(5)\log 2 - \frac{425}{64}\zeta(3)\zeta(5) - \frac{12125}{256}\zeta^2(5) + \frac{6223}{256}\zeta(7) \\
&\quad - \frac{11515}{64}\zeta(7)\log 2 + \frac{42777}{512}\zeta(3)\zeta(7)
\end{aligned}
$$

and a much more complicated expression for *P*(6). Run times increase very rapidly with the dimension *n*:

n	Digits	Processors	Run Time
2	120	1	10 sec.
3	120	8	55 min.
4	60	64	27 min.
5	30	256	39 min.
6	6	256	59 hrs.

Box Integrals

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

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

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

- $B_n(1)$ 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.

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

Recent Result (18 Jan 2009)

$$\Delta_3(-1) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{(-1 + e^{-u^2} + \sqrt{\pi}\, u \operatorname{erf}(u))^3}{u^6}\, \mathrm{d}u$$
$$= \frac{1}{15}\left(6 + 6\sqrt{2} - 12\sqrt{3} - 10\pi + 30\log(1+\sqrt{2}) + 30\log(2+\sqrt{3})\right)$$

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.

DHB, J. M. Borwein and R. E. Crandall, “Advances in the theory of box integrals,” manuscript, Mar 2009, available at 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).

Recent Evaluations of Box Integrals, Continued

n	s	$\Delta_n(s)$
2	-5	$\frac{4}{3}+\frac{8}{9}\sqrt{2}$
2	-1	$\frac{4}{3}-\frac{4}{3}\sqrt{2}+4\log(1+\sqrt{2})$
2	1	$\frac{2}{15}+\frac{1}{15}\sqrt{2}+\frac{1}{3}\log(1+\sqrt{2})$
3	-7	$\frac{4}{5}-\frac{16\sqrt{2}}{15}+\frac{2\sqrt{3}}{5}+\frac{\pi}{15}$
3	–2	$2\pi-12\ G+12\,\mathrm{Ti}_2\left(3-2\sqrt{2}\right)+6\pi\log\left(1+\sqrt{2}\right)+2\log 2-\frac{5}{2}\log 3-8\sqrt{2}\arctan\left(\frac{1}{\sqrt{2}}\right)$
3	-1	$\frac{2}{5}-\frac{2}{3}\pi+\frac{2}{5}\sqrt{2}-\frac{4}{5}\sqrt{3}+2\log\left(1+\sqrt{2}\right)+12\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)-4\log\left(2+\sqrt{3}\right)$
3	1	$-\frac{118}{21}-\frac{2}{3}\pi+\frac{34}{21}\sqrt{2}-\frac{4}{7}\sqrt{3}+2\log\left(1+\sqrt{2}\right)+8\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)$
3	3	$-\frac{1}{105}-\frac{2}{105}\pi+\frac{73}{840}\sqrt{2}+\frac{1}{35}\sqrt{3}+\frac{3}{56}\log\left(1+\sqrt{2}\right)+\frac{13}{35}\log\left(\frac{1+\sqrt{3}}{\sqrt{2}}\right)$

Recent Evaluations of Box Integrals, Continued

n	s	$\Delta_n(s)$
4	-10	$-\frac{8}{45}\pi\sqrt{3}-\frac{20}{9}\pi\log(2)+\frac{4}{9}\pi^2+\frac{4}{3}\log(2)+\frac{1}{15}\log(3)+\frac{8}{3}\mathrm{Ti}_2\left(3-2\sqrt{2}\right)$
4	-9	$\frac{16}{5}\pi\sqrt{3}-\frac{32}{3}\pi\log(2)-\frac{2}{3}\pi^2+\frac{16}{5}\pi+8\sqrt{2}\arctan\left(2\sqrt{2}\right)-24\log(2)+\frac{2}{5}\log(3)$ $+12\pi\log\left(\sqrt{2}-1\right)-64\,\mathrm{Ti}_2\left(3-2\sqrt{2}\right)+\frac{160}{3}G$
4	-3	$-\frac{128}{15}+\frac{1}{63}\pi-8\log\left(1+\sqrt{2}\right)-32\log\left(1+\sqrt{3}\right)+16\log(2)+20\log(3)$ $-\frac{8}{5}\sqrt{2}+\frac{32}{5}\sqrt{3}-32\sqrt{2}\arctan\left(\frac{1}{\sqrt{8}}\right)-96\,\mathrm{Ti}_2\left(3-2\sqrt{2}\right)+32\,G$
4	-2	$-\frac{16}{15}\pi\sqrt{3}+\frac{16}{3}\pi\log\left(1+\sqrt{3}\right)-\frac{8}{3}\pi\log(2)+4\pi\log\left(\sqrt{2}+1\right)-\frac{2}{3}\pi^2+\frac{4}{5}\pi$ $+\frac{8}{5}\sqrt{2}\arctan\left(2\sqrt{2}\right)+\frac{2}{5}\log(3)+8\,\mathrm{Ti}_2\left(3-2\sqrt{2}\right)-\frac{40}{3}G$
4	-1	$\frac{704}{195}-\frac{8}{39}\pi-\frac{100}{13}\log(3)+\frac{120}{13}\log(2)-\frac{8}{65}\sqrt{2}+\frac{128}{65}\sqrt{3}$ $-\frac{140}{13}\log\left(1+\sqrt{2}\right)-\frac{32}{13}\log\left(1+\sqrt{3}\right)+\frac{160}{13}\sqrt{2}\arctan\left(\frac{1}{\sqrt{8}}\right)+\frac{48}{13}G$
4	1	$-\frac{23}{135}-\frac{16}{315}\pi-\frac{52}{105}\log(2)+\frac{197}{420}\log(3)+\frac{73}{630}\sqrt{2}+\frac{8}{105}\sqrt{3}$ $+\frac{1}{14}\log\left(1+\sqrt{2}\right)+\frac{104}{105}\log\left(1+\sqrt{3}\right)-\frac{68}{105}\sqrt{2}\arctan\left(\frac{1}{\sqrt{8}}\right)-\frac{4}{15}G+\frac{4}{5}\mathrm{Ti}_2\left(3-2\sqrt{2}\right)$
5	-3	$-\frac{12304}{63}-\frac{512}{21}\sqrt{2}+\frac{576}{7}\sqrt{3}+\frac{800}{21}\sqrt{5}-\frac{320}{3}B_2(3)+\frac{448}{3}B_2(5)$ $-320\,B_3(1)+960\,B_3(3)-\frac{1792}{3}B_3(5)-160\,B_4(-1)+\frac{4400}{3}B_4(1)-\frac{20720}{9}B_4(3)$ $+896\,B_4(5)+32\,B_5(-3)+\frac{800}{3}B_5(-1)-1488\,B_5(1)+\frac{14336}{9}B_5(3)-448\,B_5(5)$
5	-1	$\frac{16388}{189}+\frac{1024}{189}\sqrt{2}-\frac{192}{7}\sqrt{3}-\frac{4000}{189}\sqrt{5}+\frac{64}{3}B_2(5)-\frac{192}{7}B_2(7)+\frac{320}{3}B_3(3)$ $-256\,B_3(5)+\frac{960}{7}B_3(7)+160\,B_4(1)-\frac{6160}{9}B_4(3)+784\,B_4(5)-\frac{1760}{7}B_4(7)$ $+32\,B_5(-1)-400\,B_5(1)+\frac{8192}{9}B_5(3)-672\,B_5(5)+\frac{1056}{7}B_5(7)$
5	1	$-\frac{1279}{567}G-\frac{4}{189}\pi+\frac{4}{315}\pi^2-\frac{449}{3465}+\frac{3239}{62370}\sqrt{2}+\frac{568}{3465}\sqrt{3}-\frac{380}{6237}\sqrt{5}$ $+\frac{295}{252}\log(3)+\frac{1}{54}\log\left(1+\sqrt{2}\right)+\frac{20}{63}\log\left(2+\sqrt{3}\right)+\frac{64}{189}\log\left(\frac{1+\sqrt{5}}{2}\right)$ $-\frac{73}{63}\sqrt{2}\arctan\left(\frac{1}{\sqrt{8}}\right)-\frac{8}{21}\sqrt{3}\arctan\left(\frac{1}{\sqrt{15}}\right)+\frac{104}{63}\log\left(2-\sqrt{3}\right)\theta$ $+\frac{5}{7}\mathrm{Ti}_2\left(3-2\sqrt{2}\right)+\frac{104}{63}\mathrm{Cl}_2\left(\frac{1}{3}\theta+\frac{1}{3}\pi\right)-\frac{104}{63}\mathrm{Cl}_2\left(\frac{1}{3}\theta-\frac{1}{6}\pi\right)$ $-\frac{104}{189}\mathrm{Cl}_2\left(\theta+\frac{1}{6}\pi\right)-\frac{208}{189}\mathrm{Cl}_2\left(\theta+\frac{4}{3}\pi\right)+\frac{104}{189}\mathrm{Cl}_2\left(\theta+\frac{5}{3}\pi\right)+\frac{208}{189}\mathrm{Cl}_2\left(\theta+\frac{11}{6}\pi\right)$

Cautionary Example

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

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

$$0.392699081698724154807830422909937860524645434187231595926$$

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

$$0.392699081698724154807830422909937860524646174921888227621$$

Richard Crandall has now shown that this integral is merely the first term of a very rapidly convergent series that converges to π/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.

Summary

- Numerous state-of-the-art large-scale scientific calculations now require numerical precision beyond conventional 64-bit floating-point arithmetic.
- The emerging “experimental” methodology in mathematics and mathematical physics often requires hundreds or even thousands of digits of precision.
- Double-double, quad-double and arbitrary precision software libraries are now widely available (and in most cases are free). High-precision arithmetic is also integrated into *Mathematica* and *Maple*.
- High-precision evaluation of integrals, followed by constant-recognition techniques, has been a particularly fruitful area of recent research, with many new results in pure math and mathematical physics.
- There is a critical need to develop faster techniques for high-precision numerical integration in multiple dimensions.

Summation Exercises

(a) $$\sum_{0}^{\infty} \frac{50n-6}{2^n \binom{3n}{n}}$$

(b) $$\sum_{0}^{\infty} \frac{2^{n+1}}{\binom{2n}{n}}$$

(c) $$\sum_{0}^{\infty} \frac{12n2^{2n}}{\binom{4n}{2n}}$$

(d) $$\sum_{0}^{\infty} \frac{(4n)!(1+8n)}{4^{4n}n!^4 3^{2n+1}}$$

(e) $$\sum_{0}^{\infty} \frac{275n-158}{2^n \binom{3n}{n}}$$

(f) $$\sum_{1}^{\infty} \frac{\binom{2n}{n}}{n^2 4^n}$$

(g) $$\sum_{1}^{\infty} \frac{(-1)^n}{n^3 2^n \binom{2n}{n}}$$

(h) $$\sum_{0}^{\infty} \frac{(-1)^n}{3n+1}$$

(i) $$\sum_{0}^{\infty} \frac{(-1)^n}{(n+1)^2}$$

(j) $$\sum_{0}^{\infty} \frac{(-1)^n}{(n+1)^3}$$

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

Answers are simple expressions involving rationals, π, e, sqrt(2), sqrt(3), log 2, zeta(3), Catalan's constant, Euler's constant, etc. Some can be done symbolically, but the intent here is to use numerical methods to evaluate, then use PSLQ (or similar facility) to recognize.

Integration Exercises

(a) $$\int_0^1 \frac{x^2\,dx}{(1+x^4)\sqrt{1-x^4}}$$

(b) $$\int_0^\infty xe^{-x}\sqrt{1-e^{-2x}}\,dx$$

(c) $$\int_0^\infty \frac{x^2\,dx}{\sqrt{e^x-1}}$$

(d) $$\int_0^{\pi/4} x\tan x\,dx$$

(e) $$\int_0^{\pi/2} \frac{x^2\,dx}{1-\cos x}$$

(f) $$\int_0^{\pi/4} (\pi/4 - x\tan x)\tan x\,dx$$

(g) $$\int_0^{\pi/2} \frac{x^2\,dx}{\sin^2 x}$$

(h) $$\int_0^{\pi/2} \log^2(\cos x)\,dx$$

(i) $$\int_0^1 \frac{\log^2 x\,dx}{x^2+x+1}$$

(j) $$\int_0^1 \frac{\log(1+x^2)\,dx}{x^2}$$

(k) $$\int_0^\infty \frac{\log(1+x^3)\,dx}{1-x+x^2}$$

(l) $$\int_0^\infty \frac{\log x\,dx}{\cosh^2 x}$$

(m) $$\int_0^1 \frac{\arctan x}{x\sqrt{1-x^2}}$$

(n) $$\int_0^{\pi/2} \sqrt{\tan t}\,dt$$

Answers are simple expressions involving rationals, π, e, sqrt(2), sqrt(3), log 2, zeta(3), Catalan's constant, Euler's constant, etc. Some can be done symbolically, but the intent here is to use numerical methods to evaluate, then use PSLQ (or similar facility) to recognize.

Online Resources for High-Precision Arithmetic and Experimental Math

- Experimental math website: http://www.experimentalmath.info
  Contains information and many links on experimental math.
- Inverse Symbolic Calculator, version 2: http://ddrive.cs.dal.ca/~isc/
  Online numeric constant recognition facility.
- LBNL's high-precision software: http://crd.lbl.gov/~dhbailey/mpdist
  Includes double-double, quad-double and arbitrary precision packages (C++ and Fortran-90). Also includes quadrature and PSLQ codes.
- Online experimental math toolkit: https://nebula.lbl.gov/cgi-bin/login.py
  Includes high-precision arithmetic, quadrature and PSLQ.
- *Mathematica* implementation of PSLQ:
  http://crd.lbl.gov/~dhbailey/mpdist/pslq-code.nb
- *Mathematica* solutions of exercises:
  http://crd.lbl.gov/~dhbailey/mpdist/sum-exercises.nb
  http://crd.lbl.gov/~dhbailey/mpdist/integral-exercises.nb