Computational Discovery of Number Theory Identities for Mathematical Physics Integrals

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Experimental math: Discovering new mathematical results by computer

- Compute various mathematical entities (limits, infinite series sums, definite integrals) to high precision, typically 100-1000 or more digits.
- Use algorithms such as PSLQ to recognize these entities in terms of well-known mathematical constants.
- When results are found experimentally, seek formal mathematical proofs of the discovered relations.

“If mathematics describes an objective world just like physics, there is no reason why inductive methods should not be applied in mathematics just the same as in physics.” – Kurt Godel
The PSLQ integer relation algorithm

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

\[
a_1 x_1 + a_2 x_2 + \cdots + a_n x_n = 0
\]

(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*.

Integer relation detection requires very high precision (at least \(n^*d\) 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.

PSLQ, continued

- PSLQ constructs a sequence of integer-valued matrices $B_n$ that reduces the vector $y = x \cdot B_n$, 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 $y$ vector suddenly drops to roughly “epsilon” (i.e. $10^{-p}$, where $p$ is the number of digits of precision).
- The size of this drop can be viewed as a “confidence level” that the relation is real and not merely a numerical artifact -- a drop of 20+ orders of magnitude almost always indicates a real relation.

Several efficient variants of PSLQ are available:
- 2-level and 3-level PSLQ: performs almost all PSLQ iterations with only double precision, updating full-precision arrays as needed. Hundreds of times faster than the original full-precision PSLQ algorithm.
- Multi-pair PSLQ: dramatically reduces the number of iterations required. Designed for parallel system, but runs faster even on 1 CPU.
Decrease of $\log_{10}(\min |y_i|)$ in multipair PSLQ run
In 1996, this new formula for \( \pi \) was found using a PSLQ program:

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

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

Recently it was proven that no base-\( n \) formulas of this type exist for \( \pi \), except \( n = 2^m \).

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

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

where \( x_j = g(hj) \) 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.

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

Ising integrals from mathematical physics

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

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

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

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

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

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

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

$$C_n = \frac{2^n}{n!} \int_0^\infty tK_0^n(t) \, dt$$

1000-digit numerical values, computed using this formula, approach a limit:

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

What is this limit? We copied the first 50 digits of this numerical value into the online Inverse Symbolic Calculator (ISC):


The result was:

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

where $\gamma$ denotes Euler’s constant.
Other Ising integral evaluations found using high-precision PSLQ

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

where \( \zeta \) is the Riemann zeta function and \( \text{Li}_n(x) \) is the polylog function. \( D_2, D_3 \) and \( D_4 \) were originally provided to us by mathematical physicist Craig Tracy, who hoped that our tools could help identify \( D_5 \).
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 it. The digits are available if anyone wishes to further explore it.
Recursions in Ising integrals

Consider the 2-parameter class of Ising integrals (which arises in QFT for odd $k$):

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

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

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

General recursions have now been found for all $n$.


Box integrals

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

\[ B_n(s) := \int_0^1 \cdots \int_0^1 (r_1^2 + \cdots + r_n^2)^{s/2} \, dr_1 \cdots dr_n \]

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

- \( B_n(1) \) 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.

Evaluations of box integrals

<table>
<thead>
<tr>
<th>$n$</th>
<th>$s$</th>
<th>$B_n(s)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>any</td>
<td>even $s \geq 0$</td>
<td>rational, e.g., $B_2(2) = 2/3$</td>
</tr>
<tr>
<td>1</td>
<td>$s \neq -1$</td>
<td>$\frac{1}{s+1}$</td>
</tr>
<tr>
<td>2</td>
<td>-4</td>
<td>$-\frac{1}{4} - \frac{\pi}{8}$</td>
</tr>
<tr>
<td>2</td>
<td>-3</td>
<td>$-\sqrt{2}$</td>
</tr>
<tr>
<td>2</td>
<td>-1</td>
<td>$2 \log(1 + \sqrt{2})$</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>$\frac{\sqrt{2}}{3} + \frac{3}{5} \log(1 + \sqrt{2})$</td>
</tr>
<tr>
<td>2</td>
<td>3</td>
<td>$\frac{7}{20} \log(1 + \sqrt{2})$</td>
</tr>
<tr>
<td>2</td>
<td>$s \neq -2$</td>
<td>$\frac{2}{2+s} , _2F_1\left(\frac{1}{2}, -\frac{s}{2}; \frac{3}{2}; -1\right)$</td>
</tr>
<tr>
<td>3</td>
<td>-5</td>
<td>$-\frac{1}{6} \sqrt{3} - \frac{1}{12} \pi$</td>
</tr>
<tr>
<td>3</td>
<td>-4</td>
<td>$-\frac{3}{2} \sqrt{2} \arctan \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>3</td>
<td>-2</td>
<td>$-3G + \frac{3}{2} \pi \log(1 + \sqrt{2}) + 3 , Ti_2(3 - 2\sqrt{2})$</td>
</tr>
<tr>
<td>3</td>
<td>-1</td>
<td>$-\frac{1}{4} \pi + \frac{3}{2} \log(2 + \sqrt{3})$</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>$\frac{1}{4} \sqrt{3} - \frac{1}{24} \pi + \frac{1}{2} \log(2 + \sqrt{3})$</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>$\frac{2}{5} \sqrt{3} - \frac{1}{60} \pi - \frac{7}{20} \log(2 + \sqrt{3})$</td>
</tr>
</tbody>
</table>

Here $F$ is hypergeometric function; $G$ is Catalan; $Ti$ is Lewin’s inverse-tan function.
Elliptic function integrals

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

\[ I(n_0, n_1, n_2, n_3, n_4) := \int_0^1 x^{n_0} K^{n_1}(x) K'^{n_2}(x) E^{n_3}(x) E'^{n_4}(x) dx, \]

where \( K, K', E, E' \) are elliptic integral functions:

\[ K(x) := \int_0^1 \frac{dt}{\sqrt{(1 - t^2)(1 - x^2 t^2)}} \]
\[ K'(x) := K(\sqrt{1 - x^2}) \]
\[ E(x) := \int_0^1 \frac{\sqrt{1 - x^2 t^2}}{\sqrt{1 - t^2}} dt \]
\[ E'(x) := E(\sqrt{1 - x^2}) \]

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:

\[ 81 \int_0^1 x^3 K^2(x) E(x) \, dx \equiv -6 \int_0^1 K^3(x) \, dx - 24 \int_0^1 x^2 K^3(x) \, dx \]

\[ + 51 \int_0^1 x^3 K^3(x) \, dx + 32 \int_0^1 x^4 K^3(x) \, dx \]

\[ -243 \int_0^1 x^3 K(x) E(x) K'(x) \, dx \equiv -59 \int_0^1 K^3(x) \, dx + 468 \int_0^1 x^2 K^3(x) \, dx \]

\[ + 156 \int_0^1 x^3 K^3(x) \, dx - 624 \int_0^1 x^4 K^3(x) \, dx - 135 \int_0^1 x K(x) E(x) K'(x) \, dx \]

\[ -20736 \int_0^1 x^4 E^2(x) K'(x) \, dx \equiv 3901 \int_0^1 K^3(x) \, dx - 3852 \int_0^1 x^2 K^3(x) \, dx \]

\[ -1284 \int_0^1 x^3 K^3(x) \, dx + 5136 \int_0^1 x^4 K^3(x) \, dx - 2592 \int_0^1 x^2 K^2(x) K'(x) \, dx \]

\[ -972 \int_0^1 K(x) E(x) K'(x) \, dx - 8316 \int_0^1 x K(x) E(x) K'(x) \, dx. \]
Lattice sums arising from the Poisson equation have been studied widely in mathematical physics and also in image processing.

In two 2012 papers (below), we numerically discovered, and then proved, that for rational \((x, y)\), the two-dimensional Poisson potential function satisfies

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

where \(\alpha\) is an \textit{algebraic number}, i.e., the root of an integer polynomial:

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

The minimal polynomials for these \(\alpha\) were found by PSLQ calculations, with the \((n+1)\)-long vector \((1, \alpha, \alpha^2, \ldots, \alpha^n)\) as input, where \(\alpha = \exp(\pi \phi_2(x,y))\).

PSLQ returns the vector of integer coefficients \((a_0, a_1, a_2, \ldots, a_n)\) as output.

Samples of minimal polynomials found by PSLQ

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

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

The minimal polynomial for \( \exp(8 \pi \phi_2(1/32,1/32)) \) has degree 128, with individual coefficients ranging from 1 to over \( 10^{56} \). This PSLQ computation required 10,000-digit precision. See next slide.
Jones Kimberley noted that $m(d)$ empirically satisfies:

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

where $m(2) = 1/2$, and for odd primes,

$m(4k+1) = (2k)^2$

$m(4k+3) = (2k+2)(2k+1)$
Degree-128 minimal polynomial for exp \((8 \pi \phi_2(1/32, 1/32))\)
These constants agree to 42 decimal digit accuracy, but are NOT equal:

\[ \int_0^\infty \cos(2x) \prod_{n=1}^\infty \cos(x/n) \, dx = \]

\[ 0.392699081698724154807830422909937860524645434187231595926 \]

\[ \frac{\pi}{8} = \]

\[ 0.392699081698724154807830422909937860524646174921888227621 \]

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

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


Summary

- High-precision numerical computation has emerged as a very powerful tool for discovery in mathematical research.
- Some research studies, particularly in problems that arise in mathematical physics, require hundreds or even thousands of digits.
- The key algorithms for this research are:
  - The tanh-sinh quadrature algorithm, which readily handles many functions with integral singularities, and which scales to thousands of digits.
  - The PSLQ integer relation algorithm, which discovers underlying identities for the given constant in terms of a linear sum of conjectured terms (or as relations among such computed entities).
- Even though such computations often provide dramatic and convincing evidence for an assertion, they do not constitute rigorous proof – this must be done the “old-fashioned” way.

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