Computation and experimental evaluation of Mordell–Tornheim–Witten sum derivatives

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The PSLQ integer relation algorithm

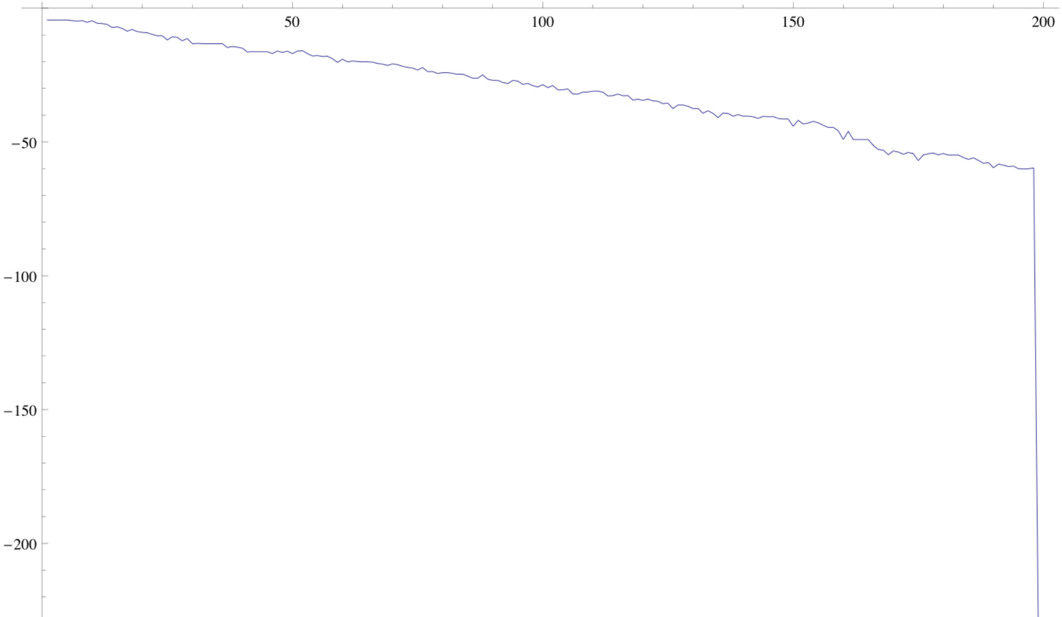
Let $X = (x_k)$ be an $(m+1)$-long real or complex vector. An integer relation algorithm such as PSLQ finds a nontrivial integer vector $A = (a_k)$ such that

$$a_0 x_0 + a_1 x_1 + \cdots + a_m x_m \quad = \quad 0.$$

- The multipair PSLQ algorithm is a more efficient and parallelizable variant of PSLQ, the most widely used integer relation algorithm (other researchers use a variant of the LLL algorithm).
- Integer relation detection (by any algorithm) requires very high precision: at least $(m+1) \cdot \max_k \log_{10} |a_k|$ digits, both in the input data and the algorithm.

- 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.
- D. H. Bailey and D. J. Broadhurst, "Parallel integer relation detection: Techniques and applications," *Mathematics of Computation*, vol. 70, no. 236 (Oct 2000), 1719–1736.

Decrease of $\log 10(\min |y_i|)$ in multipair PSLQ run



Application of multipair PSLQ

One simple but important application of multipair PSLQ is to recognize a computed numerical value as the root of an integer polynomial of degree m.

Example: The following constant is suspected to be an algebraic number:

$\alpha = 1.232688913061443445331472869611255647068988824547930576057634684778\ldots$

What is its minimal polynomial?

Method: Compute the vector $(1, \alpha, \alpha^2, \cdots, \alpha^m)$ for $m = 30$, then input this vector to multipair PSLQ.

Answer (using 250-digit arithmetic):

$$\begin{aligned} 0 = {} & 697 - 1440\alpha - 20520\alpha^2 - 98280\alpha^3 - 102060\alpha^4 - 1458\alpha^5 + 80\alpha^6 - 43920\alpha^7 \\ & + 538380\alpha^8 - 336420\alpha^9 + 1215\alpha^{10} - 80\alpha^{12} - 56160\alpha^{13} - 135540\alpha^{14} - 540\alpha^{15} \\ & + 40\alpha^{18} - 7380\alpha^{19} + 135\alpha^{20} - 10\alpha^{24} - 18\alpha^{25} + \alpha^{30} \end{aligned}$$

The Poisson potential function

In 2012, Richard Crandall, while investigating techniques to sharpen images, noted that each pixel was given by a form of the 2-D Poisson potential function:

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

In a 2013 study, we numerically discovered, and then proved the intriguing fact that for rational (x, y),

$$\phi_2(x, y) = \frac{1}{\pi} \log \alpha$$

where α is *algebraic*, i.e., the root of a some integer polynomial of degree m.

By computing high-precision numerical values of $\phi_2(x, y)$ for various specific rational x and y, and applying a multipair PSLQ program, we were able to produce the explicit minimal polynomials for α in numerous specific cases.

- D. H. Bailey, J. M. Borwein, R. E. Crandall and J. Zucker, "Lattice sums arising from the Poisson equation," *Journal of Physics A: Mathematical and Theoretical*, vol. 46 (2013), 115201.

Samples of minimal polynomials found by multipair PSLQ

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

These computations are very expensive. The case $x = y = 1/32$, for instance, required 10,000-digit arithmetic and ran for 45 hours. Other runs, using even higher precision, ultimately failed, evidently due to subtle program bugs. Help!

Kimberley's formula for the degree of the polynomial

Based on our preliminary results, Jason Kimberley of the University of Newcastle, Australia observed that the degree $m(s)$ of the minimal polynomial associated with the case $x = y = 1/s$ appears to be given by the following:

Set $m(2) = 1/2$. Otherwise for primes p congruent to 1 mod 4, set $m(p) = \mathrm{int}^2(p/2)$, where int denotes greatest integer, and for primes p congruent to 3 mod 4, set $m(p) = \mathrm{int}\,(p/2)(\mathrm{int}\,(p/2) + 1)$. Then for any other positive integer s whose prime factorization is $s = p_1^{e_1} p_2^{e_2} \cdots p_r^{e_r}$,

$$m(s) \stackrel{?}{=} 4^{r-1} \prod_{i=1}^{r} p_i^{2(e_i-1)}\, m(p_i).$$

Does Kimberley's formula hold for larger s? Why?

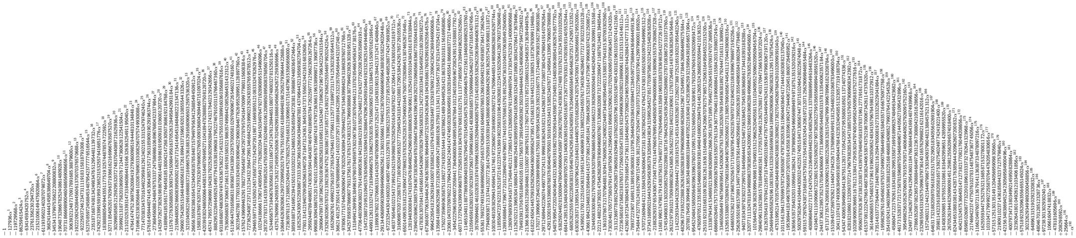
What is the true mathematical connection between the pair of rationals (x, y) and the algebraic number α?

Three improvements to the Poisson polynomial computation program

1. MPFUN2015: A new thread-safe multiprecision package.
   - Speedup: 3X
2. A new 3-level multipair PSLQ program.
   - Speedup: 4.2X
3. Parallel implementation on a 16-core system.
   - Speedup: 12.2X

Overall speedup: 156X

192-degree minimal polynomial found by multipair PSLQ for $x = y = 1/35$



This polynomial has degree 192, with coefficients as large as 10^{85}. This computation required 18,000-digit arithmetic and 34 CPU-hours.

The case $(1/37, 1/37)$ required 51,000-digit arithmetic and 90 CPU-days (5.6 days on a 16-core parallel system).

Kimberley's formula was upheld for $(1/s, 1/s)$, for all s up to 52 (except for $s = 41, 43, 47, 49, 51$, which were too expensive), and also for $s = 60$ and $s = 64$.

Palindromic polynomials

From our results, in the case $(1/s, 1/s)$ where s is even, the resulting polynomial is always palindromic ($a_k = a_{m-k}$). For instance, when $s = 16$,

$$\begin{aligned}
p_{16}(\alpha) = 1 &- 1376\alpha^1 - 12560\alpha^2 - 3550496\alpha^3 + 81241720\alpha^4 - 169589984\alpha^5 \\
&+ 1334964944\alpha^6 - 24307725984\alpha^7 + 238934926108\alpha^8 - 1043027124704\alpha^9 \\
&+ 2328675366384\alpha^{10} - 3219896325280\alpha^{11} + 4238551472456\alpha^{12} \\
&- 10247414430048\alpha^{13} + 28552105805904\alpha^{14} - 55832851687968\alpha^{15} \\
&+ 70020268309062\alpha^{16} \\
&- 55832851687968\alpha^{17} + 28552105805904\alpha^{18} - 10247414430048\alpha^{19} \\
&+ 4238551472456\alpha^{20} - 3219896325280\alpha^{21} + 2328675366384\alpha^{22} \\
&- 1043027124704\alpha^{23} + 238934926108\alpha^{24} - 24307725984\alpha^{25} + 1334964944\alpha^{26} \\
&- 169589984\alpha^{27} + 81241720\alpha^{28} - 3550496\alpha^{29} - 12560\alpha^{30} - 1376\alpha^{31} + \alpha^{32}
\end{aligned}$$

Nitya Mani, an undergraduate student at Stanford University, observed that if α is a root of a palindromic polynomial such as this, then $\alpha + 1/\alpha$ is a root of a transformed polynomial of half the degree. This fact can be used to significantly accelerate the computation of Poisson polynomials in the even case.

Proofs of Kimberley's formula and the palindromic property

- On March 16, DHB presented our results at a seminar at the University of California, Berkeley.
- Following the presentation, Watson Ladd, a graduate student in mathematics, brought to our attention the fact that some of our conjectures should follow from results in the theory of elliptic curves, Gaussian integers and ideals.
- After some effort, Ladd produced proofs of Kimberley's formula and the palindromic property, which proofs were then incuded in our paper and returned to the journal.
- The paper has now appeared:
  David H. Bailey, Jonathan M. Borwein, Jason Kimberley and Watson Ladd, "Computer discovery and analysis of large Poisson polynomials," *Experimental Mathematics*, 27 Aug 2016.
- A preprint is available here:
  `http://www.davidhbailey.com/dhbpapers/poisson-res.pdf`.

Mordell–Tornheim–Witten sums

The simplest MTW sum is:

$$W(r,s,t) = \sum_{m,n\geq 1} \frac{1}{m^r n^s (m+n)^t}.$$

Such sums arise in combinatorics, mathematical physics (e.g., Feynmann diagrams and string theory), Lie algebras, number theory and numerous other fields. In special cases these sums have simple evaluations. For example, when $t = 0$,

$$W(r,s,0) = \sum_{m,n\geq 1} \frac{1}{m^r n^s} = \sum_{m\geq 1} \frac{1}{m^r} \sum_{n\geq 1} \frac{1}{n^s} = \zeta(r)\zeta(s).$$

The n-dimensional MTW sum is defined for integer m_i and positive real r_i as

$$W(r_1, r_2, \ldots, r_n, t) = \sum_{m_1,\ldots,m_n \geq 1} \frac{1}{m_1^{r_1} m_2^{r_2} \cdots m_n^{r_n} (m_1 + m_2 + \cdots + m_n)^t}.$$

Matsumoto proved that W can be continued meromorphically to the entire $\mathbb{C}^{r+1}$ space.

Special case

We will focus on the special case $r_1 = r_2 = \cdots = r_n = t = s$ for real s (analytically continued as above), namely

$$\omega_{n+1}(s) = \sum_{m_1, m_2, \ldots, m_n \geq 1} \frac{1}{(m_1 m_2 \cdots m_n (m_1 + m_2 + \cdots + m_n))^s},$$

for $n = 2, 3, \cdots$. These sums were studied by Tomkins, who conjectured that

$$\omega_{n+1}(0) = \frac{(-1)^n}{n+1}.$$

This was proved by Romik for the case $n = 2$ and in the general case by Borwein and Dilcher.

1. H. Tomkins, “An exploration of multiple zeta functions,” Honours Thesis, Dalhousie University, 21 Apr 2016.
2. J. M. Borwein and K. Dilcher, “Derivatives and fast evaluation of multiple Witten functions,” manuscript, to appear in *Ramanujan Journal*, 2016.
3. D. Romik, “On the number of n-dimensional representations of $SU(3)$, the Bernoulli numbers, and the Witten zeta function,” 17 Apr 2015, `https://arxiv.org/pdf/1503.03776v3.pdf`.

Key result from Tomkins' thesis

Let $r_1, r_2, \ldots, r_n, t$ be complex variables with $r_i \in \mathbb{N}$ for $1 \leq i \leq n$. Then for any real $\theta > 0$,

$$\Gamma(t)W(r_1, r_2, \ldots, r_n, t) = \sum_{m_1, m_2, \ldots m_n \geq 1} \frac{\Gamma(t, (m_1 + m_2 + \cdots + m_n)\theta)}{m_1^{r_1} m_2^{r_2} \cdots m_n^{r_n} (m_1 + m_2 + \cdots + m_n)^t}$$

$$+ \sum_{\{a_1, a_2, \ldots, a_k\} \subset \{1,2,\ldots,n\}} \left(\sum_{u_{a_1}, u_{a_2}, \ldots, u_{a_k} \geq 0} \frac{\theta^w}{w} \prod_{i=1}^{n} \Gamma(1 - r_i) \prod_{j=1}^{k} \frac{(-1)^{u_{a_j}} \zeta(r_{a_j} - u_{a_j})}{u_{a_j}!\, \Gamma(1 - r_{a_j})} \right),$$

where $w = t - (n - k) + \sum_{j=1}^{k} (u_{a_j} - r_{a_j}) + \sum_{i=1}^{n} r_i$.

Example: Special case when $n = 4$

$$\omega_4(s) = \frac{1}{\Gamma(s)} \left[\sum_{m,n,p \geq 1} \frac{\Gamma(s, (m+n+p)\theta)}{(mnp(m+n+p))^s} \right.$$
$$+ \sum_{m,n,p \geq 0} \frac{(-1)^{m+n+p} \zeta(s-m)\zeta(s-n)\zeta(s-p)\theta^{m+n+p+s}}{m!n!p!(m+n+p+s)}$$
$$+ 3\Gamma(1-s) \sum_{m,n \geq 0} \frac{(-1)^{m+n} \zeta(s-m)\zeta(s-n)\theta^{m+n+2s-1}}{m!n!(m+n+2s-1)}$$
$$\left. +3(\Gamma(1-s))^2 \sum_{p \geq 0} \frac{(-1)^p \zeta(s-p)\theta^{p+3s-2}}{p!(p+3s-2)} + (\Gamma(1-s))^3 \frac{\theta^{4s-3}}{4s-3} \right],$$

where $\theta > 0$ is an arbitrary real parameter, and s is real but not an integer.

Computation of ω_n derivatives

In initial computations of omega derivatives at zero, namely $\omega_d'(0)$ for $d = 3, 4, \ldots$, Borwein and Dilcher found and then proved the intriguing experimental equivalence

$$\omega_3'(0) \;=\; \log(2\pi),$$

based purely on the numerical value of $\omega_3'(0)$ as computed from a more complex evaluation due to Romik, where the sum arises in counting representations of $SU(3)$. Tomkins then showed that

$$\omega_4'(0) \;=\; -\log(2\pi) + \zeta'(-2).$$

These results immediately raise the question of whether the higher-degree constants $\omega_d'(0)$ have similarly elegant evaluations.

Numerical issues

We computed these constants to 400-digit precision and then employed the multipair PSLQ algorithm to attempt to obtain an analytic evaluation.

Straightforward evaluation is exceedingly expensive, since with each higher degree d, the summations involve one more level of loop nesting, and each higher level of loop nesting typically increases the computational run time by a factor of 10 or more over the previous level.

However, after carefully examining these formulas and the equivalent computer code, we ultimately achieved a 30-million-fold speedup.

PSLQ analysis

In this application, we defined $x_0 = \omega_d'(0)$, and then selected a set of candidate constants, based on experience with the cases degree $d = 3$ and $d = 4$. In particular, we tried the following input vectors x in our multipair PSLQ computations, where all terms are computed to at least 400-digit precision:

$$
\begin{aligned}
x &= \left(\omega_d'(0), \log(2\pi), \zeta'(-2), \zeta'(-4), \cdots, \zeta'(-d+3)\right) \quad \text{for odd } d \\
x &= \left(\omega_d'(0), \log(2\pi), \zeta'(-2), \zeta'(-4), \cdots, \zeta'(-d+2)\right) \quad \text{for even } d.
\end{aligned}
$$

Experimental relations produced by multipair PSLQ

$$
\begin{aligned}
0 &\doteq \omega_4'(0) + \log(2\pi) - \zeta'(-2)\\
0 &\doteq -\omega_5'(0) + \log(2\pi) - 2\,\zeta'(-2)\\
0 &\doteq 12\,\omega_6'(0) + 12\,\log(2\pi) - 35\,\zeta'(-2) - \zeta'(-4)\\
0 &\doteq 4\,\omega_7'(0) - 4\,\log(2\pi) + 15\,\zeta'(-2) + \zeta'(-4)\\
0 &\doteq -360\,\omega_8'(0) - 360\,\log(2\pi) + 1624\,\zeta'(-2) + 175\,\zeta'(-4) + \zeta'(-6)\\
0 &\doteq 90\,\omega_9'(0) - 90\,\log(2\pi) + 469\,\zeta'(-2) + 70\,\zeta'(-4) + \zeta'(-6)\\
0 &\doteq -20160\,\omega_{10}'(0) - 20160\,\log(2\pi) + 118124\,\zeta'(-2) + 22449\,\zeta'(-4) + 546\,\zeta'(-6) + \zeta'(-8)\\
0 &\doteq -4032\,\omega_{11}'(0) + 4032\,\log(2\pi) - 26060\,\zeta'(-2) - 5985\,\zeta'(-4) - 210\,\zeta'(-6) - \zeta'(-8)\\
0 &\doteq 1814400\,\omega_{12}'(0) + 1814400\,\log(2\pi) - 12753576\,\zeta'(-2) - 3416930\,\zeta'(-4)\\
&\quad -157773\,\zeta'(-6) - 1320\,\zeta'(-8) - \zeta'(-10)\\
0 &\doteq -302400\,\omega_{13}'(0) + 302400\,\log(2\pi) - 2286636\,\zeta'(-2) - 696905\,\zeta'(-4)\\
&\quad -39963\,\zeta'(-6) - 495\,\zeta'(-8) - \zeta'(-10)\\
0 &\doteq 239500800\,\omega_{14}'(0) + 239500800\,\log(2\pi) - 1931559552\,\zeta'(-2) - 657206836\,\zeta'(-4)\\
&\quad -44990231\,\zeta'(-6) - 749463\,\zeta'(-8) - 2717\,\zeta'(-10) - \zeta'(-12)\\
0 &\doteq 34214400\,\omega_{15}'(0) - 34214400\,\log(2\pi) + 292271616\,\zeta'(-2) + 109425316\,\zeta'(-4)\\
&\quad +8691683\,\zeta'(-6) + 183183\,\zeta'(-8) + 1001\,\zeta'(-10) + \zeta'(-12)\\
0 &\doteq -43589145600\,\omega_{16}'(0) - 43589145600\,\log(2\pi) + 392156797824\,\zeta'(-2) + 159721605680\,\zeta'(-4)\\
&\quad +14409322928\,\zeta'(-6) + 368411615\,\zeta'(-8) + 2749747\,\zeta'(-10) + 5005\,\zeta'(-12) + \zeta'(-14)\\
0 &\doteq 5448643200\,\omega_{17}'(0) - 5448643200\,\log(2\pi) + 51381813456\,\zeta'(-2) + 22556777880\,\zeta'(-4)\\
&\quad +2273360089\,\zeta'(-6) + 68396900\,\zeta'(-8) + 654654\,\zeta'(-10) + 1820\,\zeta'(-12) + \zeta'(-14)
\end{aligned}
$$

Solved relations

$$
\begin{aligned}
\omega_4'(0) &\mathrel{\hat{=}} -\log(2\pi) + \zeta'(-2)\\
\omega_5'(0) &\mathrel{\hat{=}} \log(2\pi) - 2\,\zeta'(-2)\\
\omega_6'(0) &\mathrel{\hat{=}} -\log(2\pi) + \frac{35\,\zeta'(-2)}{12} + \frac{\zeta'(-4)}{12}\\
\omega_7'(0) &\mathrel{\hat{=}} \log(2\pi) - \frac{15\,\zeta'(-2)}{4} - \frac{\zeta'(-4)}{4}\\
\omega_8'(0) &\mathrel{\hat{=}} -\log(2\pi) + \frac{203\,\zeta'(-2)}{45} + \frac{35\,\zeta'(-4)}{72} + \frac{\zeta'(-6)}{360}\\
\omega_9'(0) &\mathrel{\hat{=}} \log(2\pi) - \frac{469\,\zeta'(-2)}{90} - \frac{7\,\zeta'(-4)}{9} - \frac{\zeta'(-6)}{90}\\
\omega_{10}'(0) &\mathrel{\hat{=}} -\log(2\pi) + \frac{29531\,\zeta'(-2)}{5040} + \frac{1069\,\zeta'(-4)}{960} + \frac{13\,\zeta'(-6)}{480} + \frac{\zeta'(-8)}{20160}\\
\omega_{11}'(0) &\mathrel{\hat{=}} \log(2\pi) - \frac{6515\,\zeta'(-2)}{1008} - \frac{95\,\zeta'(-4)}{64} - \frac{5\,\zeta'(-6)}{96} - \frac{\zeta'(-8)}{4032}\\
\omega_{12}'(0) &\mathrel{\hat{=}} -\log(2\pi) + \frac{177133\,\zeta'(-2)}{25200} + \frac{341693\,\zeta'(-4)}{181440} + \frac{7513\,\zeta'(-6)}{86400} + \frac{11\,\zeta'(-8)}{15120} + \frac{\zeta'(-10)}{1814400}\\
\omega_{13}'(0) &\mathrel{\hat{=}} \log(2\pi) - \frac{190553\,\zeta'(-2)}{25200} - \frac{139381\,\zeta'(-4)}{60480} - \frac{1903\,\zeta'(-6)}{14400} - \frac{11\,\zeta'(-8)}{6720} - \frac{\zeta'(-10)}{302400}\\
\omega_{14}'(0) &\mathrel{\hat{=}} -\log(2\pi) + \frac{1676701\,\zeta'(-2)}{207900} + \frac{14936519\,\zeta'(-4)}{5443200} + \frac{4090021\,\zeta'(-6)}{21772800} + \frac{22711\,\zeta'(-8)}{7257600} + \frac{247\,\zeta'(-10)}{21772800}\\
&\quad + \frac{\zeta'(-12)}{239500800}\\
\omega_{15}'(0) &\mathrel{\hat{=}} \log(2\pi) - \frac{63427\,\zeta'(-2)}{7425} - \frac{2486939\,\zeta'(-4)}{777600} - \frac{790153\,\zeta'(-6)}{3110400} - \frac{5551\,\zeta'(-8)}{1036800} - \frac{91\,\zeta'(-10)}{3110400}\\
&\quad - \frac{\zeta'(-12)}{34214400}\\
\omega_{16}'(0) &\mathrel{\hat{=}} -\log(2\pi) + \frac{30946717\,\zeta'(-2)}{3439800} + \frac{21939781\,\zeta'(-4)}{5987520} + \frac{899683\,\zeta'(-6)}{2721600} + \frac{515261\,\zeta'(-8)}{60963840} + \frac{2747\,\zeta'(-10)}{43545600}\\
&\quad + \frac{\zeta'(-12)}{8709120} + \frac{\zeta'(-14)}{43589145600}\\
\omega_{17}'(0) &\mathrel{\hat{=}} \log(2\pi) - \frac{13215487\,\zeta'(-2)}{1401400} - \frac{2065639\,\zeta'(-4)}{498960} - \frac{2271089\,\zeta'(-6)}{5443200} - \frac{4783\,\zeta'(-8)}{381024} - \frac{109\,\zeta'(-10)}{907200}\\
&\quad - \frac{\zeta'(-12)}{2993760} - \frac{\zeta'(-14)}{5448643200}
\end{aligned}
$$

Problem: Can we prove these experimental relations?

- This talk is available at http://www.davidhbailey.com/dhbtalks/dhb-wcnt-2016.pdf.
- A preprint with full details, results and analysis is available at http://www.davidhbailey.com/dhbpapers/omega-numerics.pdf.