Computation of the omega function

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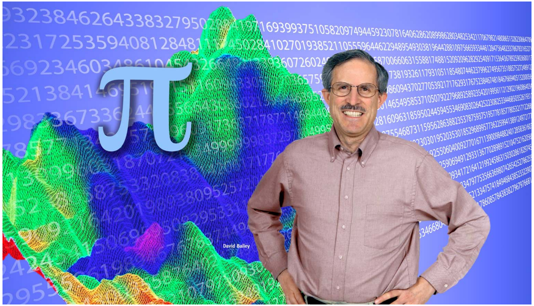


Mordell-Tornheim-Witten sums and the omega function

Mordell-Tornheim-Witten sums are defined as:

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

They can be continued analytically, as specified by Matsumoto.

Such sums arise in combinatorics, mathematical physics (e.g., Feynmann diagrams and string theory), Lie algebras, number theory and numerous other fields.

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

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

- 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`.
- H. Tomkins, "An exploration of multiple zeta functions," Honours Thesis, Dalhousie University, 21 Apr 2016.

The degree-two omega function

The degree-two instance of the omega function is

$$\omega(s) = \sum_{j,k=1}^{\infty} \frac{1}{(jk(j+k))^s}.$$

For positive integer arguments, papers by Subbarao, Sitaramachandrarao, Garoufalidis, Zagier, Huard, Williams and Nan-Yue have shown that for positive integers n,

$$\omega(2n) = \frac{4}{3} \sum_{k=0}^{n} \binom{4n-2k-1}{2n-1} \zeta(2k)\zeta(6n-2k)$$

$$\omega(2n+1) = -4 \sum_{k=0}^{n} \binom{4n-2k-1}{2n} \zeta(2k)\zeta(6n-2k+3).$$

Specific values of omega

$$\omega(1) = 2\zeta(3)$$
$$\omega(2) = \frac{1}{2835}\pi^6$$
$$\omega(3) = -2\pi^2\zeta(7) + 20\zeta(9)$$
$$\omega(4) = \frac{19}{273648375}\pi^{12}$$
$$\omega(5) = -\frac{2}{9}\pi^4\zeta(11) - \frac{70}{3}\pi^2\zeta(13) + 252\zeta(15)$$
$$\omega(6) = \frac{2062}{116937886440375}\pi^{18}$$
$$\omega(7) = -\frac{4}{135}\pi^6\zeta(15) - \frac{56}{15}\pi^4\zeta(17) - 308\pi^2\zeta(19) + 3432\zeta(21)$$
$$\omega(8) = \frac{32293}{7060124893837640625}\pi^{24}$$

Romik's formulas for omega

Dan Romik has shown that

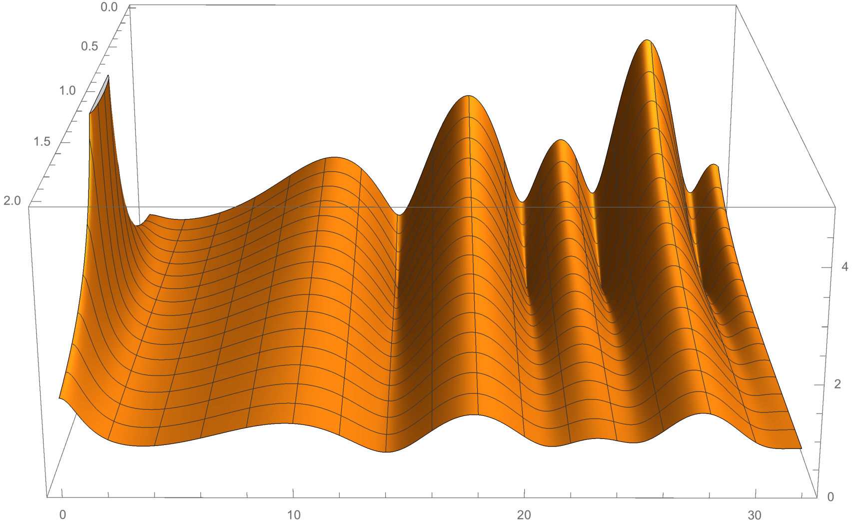
$$\omega(s) = \frac{1}{2\pi\Gamma(s)} \int_{(\alpha)} \Gamma(s+z)\Gamma(-z)\zeta(2s+z)\zeta(s-z)\,\mathrm{d}z,$$

where (α) means the vertical line $\{\alpha + ti, -\infty < t < \infty\}$. This is valid for all complex s satisfying $\max(-\mathrm{Re}(s), 1 - 2\mathrm{Re}(s)) < \alpha < \min(0, \mathrm{Re}(s) - 1)$. This can be written, avoiding singularities, as:

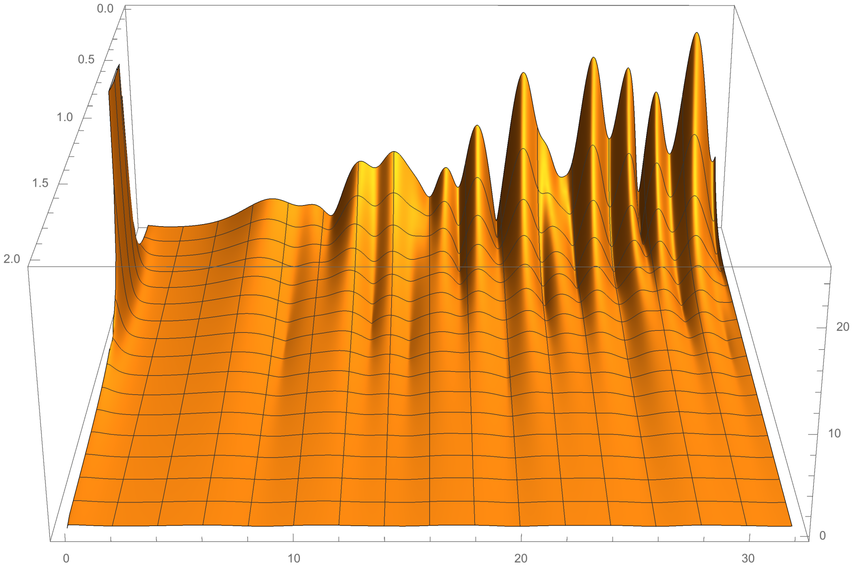
$$\begin{aligned}\omega(s) = \frac{1}{\Gamma(s)}\Bigg(&\Gamma(2s-1)\Gamma(1-s)\zeta(3s-1) \\ &+ \sum_{k=0}^{M-1} \frac{(-1)^k}{k!}\Gamma(s+k)\zeta(2s+k)\zeta(s-k) \\ &+ \frac{1}{2\pi}\int_{(\alpha)} \Gamma(s+z)\Gamma(-z)\zeta(2s+z)\zeta(s-z)\,\mathrm{d}z\Bigg).\end{aligned}$$

This is valid for all complex s satisfying $3/4 - M/2 < \mathrm{Re}(s) < M + 1/2$.

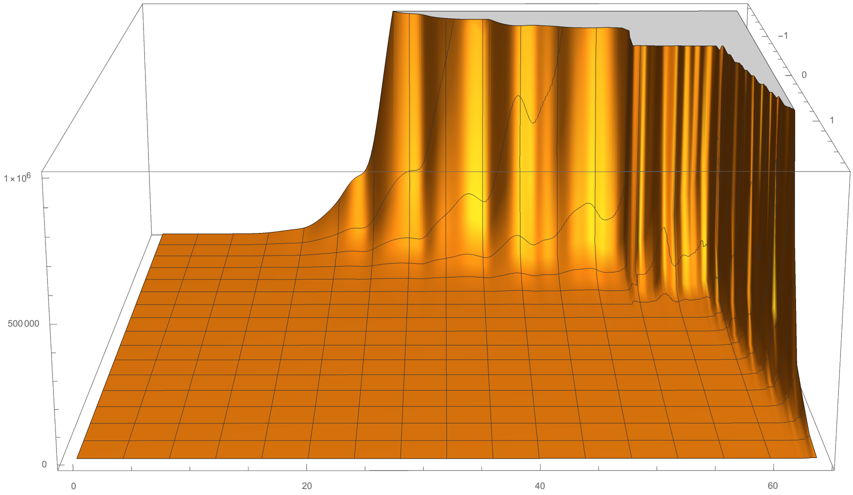
The Riemann zeta function in the complex plane



The omega function on $[x + iy, 0 \leq x \leq 2, 1/8 \leq y \leq 32]$



The omega function on $[x + iy, -2 \leq x \leq 2, 1/8 \leq y \leq 64]$



Research questions for omega

- Does omega have any zeroes in the complex plane? Where? How many?
- Does omega have nice analytic formulas for any arguments other than positive integers? Can we discover these formulas experimentally?
- Can we do a similar analysis of the derivative of omega? For higher derivatives?
- How about for higher-degree omega?

The argument principle

Note, by the argument principle, that the number of zeroes of $\omega(s)$ in a pole-free region bounded by a contour C in the complex plane can be computed as:

$$-\frac{1}{2\pi i}\int_{(C)}\frac{\omega'(s)}{\omega(s)}\,\mathrm{d}s$$

Computing the omega function

Key elements of computing $\omega(s)$ for complex s:

- Evaluating $\Gamma(s)$.
- Evaluating $\zeta(s)$.
- Evaluating Romik's integral formula.

To count zeroes in a region using the argument principle, it is also necessary to compute the derivative $\omega'(s)$. This can be done by

$$\omega'(s) \approx \frac{\omega(s+h) - \omega(s)}{h},$$

where $h = 10^{-p/2}$ and p is the working precision level in digits (yielding the derivative accurate to $p/2$ digits).

The reliability of these results strongly depends on performing the computations to convincingly high precision — more than standard 64-bit floating-point arithmetic.

Computing gamma and zeta

The best way to compute $\Gamma(s)$ is to use a formula originally due to Spouge:

$$\Gamma(1+z) \approx (z+a)^{z+1/2} e^{-z-a} \sqrt{2\pi} \left(1 + \sum_{k=1}^{\lceil a \rceil - 1} \frac{c_k(a)}{z+k}\right),$$

where $a =$ number of desired digits, and

$$c_k(a) = \frac{(-1)^{k-1}(a-k)^{k-1/2} e^{-k+a}}{\sqrt{2\pi}(k-1)!}.$$

The best way to compute $\zeta(s)$ is to use a formula due to Richard Crandall:

$$\zeta(s) = \frac{1}{\Gamma(s/2)} \left[\frac{\pi^{s/2}}{s(s-1)} + \sum_{n=1}^{\infty} \left(\frac{\Gamma(s/2, \pi n^2)}{n^s} + \frac{\pi^{s-1/2}\Gamma((1-s)/2, \pi n^2)}{n^{1-s}}\right)\right],$$

where $\Gamma(s,x)$ is the incomplete gamma function:

$$\Gamma(s,x) = \Gamma(s)\left(1 - x^s e^{-x} \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(s+k+1)}\right).$$

Computing the integral in Romik's formula using the tanh-sinh scheme

Given $f(x)$ defined on $(-1,1)$, define $g(t) = \tanh(\pi/2 \cdot \sinh t)$. Seting $x = g(t)$ 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 the abscissas x_j and the weights w_j are given by:

$$x_j = g(hj) = \tanh(\pi/2 \cdot \sinh(hj))$$
$$w_j = g'(hj) = \pi/2 \cdot \cosh(hj)/\cosh^2(\pi/2 \cdot \sinh(hj)).$$

Features:

- Halving h (i.e., doubling N) typically *doubles* the number of correct digits.
- The scheme works well even for functions with blow-up singularities at endpoints.
- The cost of computing abscissas and weights increases *linearly* with the number N of subdivisions, whereas it increases *quadratically* for most other schemes.

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

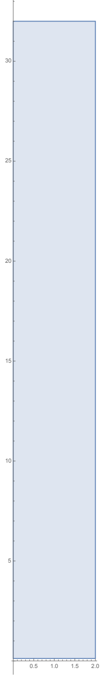
Software for high-precision computation

- Mathematica and Maple: Both feature well-integrated arbitrary precision facilities, but are often quite slow.
- Sage: Also includes arbitrary precision facility, but not as many functions.
- gfortran's quad precision: Now includes full support for `real(16)` and `complex(16)` datatypes (128-bit IEEE arithmetic, approximately 33 digits).
- GMP: GNU-supported package for arbitrary precision *integer* computation.
- MPFR: Very efficient package for arbitrary precision *floating-point* computation, built on top of GMP; does not include high-level language facilities.
- DHB's software (each includes high-level language support):
  - QD: Double-double (31 digits) and quad-double (62 digits); C++ and Fortran.
  - ARPREC: Arbitrary precision floating-point package; C++ and Fortran.
  - MPFUN2015: New Fortran arbitrary precision package, based on MPFR; Fortran.

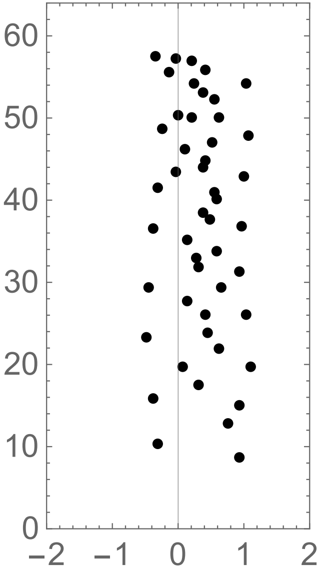
What has been done

These have been implemented, using the MPFUN2015 multiprecision software:

- Routine to compute $\Gamma(s)$ for any complex s.
- Routine to compute $\Gamma(s, x)$ for any complex s and all real x.
- Routine to compute $\zeta(s)$ for any complex s.
- Routine to compute $\omega(s)$ for any complex s, using Romik's integral formulas and the tanh-sinh quadrature algorithm (using MPFUN2015).
- Computation of the contour integral for the rectangular contour $(0, 1/8)$ to $(2, 1/8)$ to $(2, 64)$ to $(0, 64)$, and back to $(0, 1/8)$, all using 70-digit precision.



Zeroes of omega in the region $[x + iy, -2 \leq x \leq 2, 1/8 \leq y \leq 64]$



What remains to be done

- Run times are ridiculously high. Can the program be tuned to run faster? Use different high-precision software? Run on a parallel system?
- Can a much larger range of complex arguments be explored, looking for zeroes, perhaps not necessarily using the argument principle?
- Can we do the same for the derivative of omega or higher-order derivatives? Can we do the same for higher-degree omega?

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This talk is available at:
http://www.davidhbailey.com/dhbtalks/dhb-wcnt-2017.pdf