Computation and theory of Mordell-Tornheim-Witten sums II

(Dedicated to Richard Askey on the occasion of his eightieth birthday)

D. H. Bailey* J. M. Borwein†

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Abstract

In [8] the current authors, along with the late and much-missed Richard Crandall (1947–2012), considered generalized Mordell–Tornheim–Witten (MTW) zeta-function values along with their derivatives, and explored connections with multiple-zeta values (MZVs). This entailed use of symbolic integration, high precision numerical integration, and some interesting combinatorics and special-function theory. The original motivation was to represent objects such as Eulerian log-gamma integrals; and all such integrals were expressed in terms of a MTW basis. Herein, we extend the research envisaged in [8] by analyzing the relations between a significantly more general class of MTW sums. This has required significantly more subtle scientific computation and concomitant special function theory.

1 Introduction

In [8] we defined an ensemble of extended Mordell–Tornheim–Witten (MTW) zeta function values [23, 36, 29, 30, 5, 15, 37, 38]. There is by now a huge literature on these sums; in part because of the many connections with fields such as combinatorics, number theory, and mathematical physics. Unlike previous authors we included *derivatives with respect to the order* of the terms. We investigated interrelations between MTW evaluations, and explored some deeper connections with multiple-zeta values (MZVs). To achieve these results, we used symbolic and numerical integration, special function theory and some less-than-obvious combinatorics and generating function analysis.

Our original motivation was that of representing previously unresolved constructs such as Eulerian log-gamma integrals

$$\mathcal{L}G_n \ := \ \int_0^1 \log^n \Gamma(x)\,\mathrm{d}x.$$

For that purpose it was necessary to consider only one differentiation of $\mathrm{Li}_s(z)$ with respect to s—though the requisite tools for higher order derivatives were laid out in [8]. For additional introductory material we refer to [8]. These approaches are extended to character polylogarithms in [6]. Some related results and computational algorithms for the incomplete gamma function, the Hurwitz zeta function, and the Dirichlet L-series are presented in [7].

*Lawrence Berkeley National Lab (retired), Berkeley, CA 94720, and University of California, Davis, Dept. of Computer Science, Davis, CA 95616, USA. E-mail: david@davidhbailey.com.

†CARMA, University of Newcastle NSW 2303, Australia, E-mail: jon.borwein@gmail.com

In this article we continue the research envisaged in [8] by analyzing the relations between higher-order MTW sums. This paper is, in consequence, in part in homage to our friend and collaborator Richard Crandall who died after a short illness on December 20, 2012. It is also a fitting tribute to Dick Askey, whose role in the development of modern special function theory has been prodigious (see [1] and the discussion in [19]). In *Indiscrete Thoughts* [34, p. 216] Gian-Carlo Rota writes "special functions [is] a Wisconsin subject," but in this setting 'Askey' is a synonym for 'Wisconsin'.

1.1 Organization

The organization of the paper is as follows. In Section 2 we recall an ensemble $\mathcal{D}$ capturing the values we wish to study and provide effective integral representations in terms of polylogarithms on the unit circle. (In Section 4.5 we reprise a subensemble $\mathcal{D}_1$ sufficient for the study log gamma integrals.) In Section 3 we provide the necessary polylogarithmic algorithms for computation of our sums/integrals to high precision (400 digits up to 3100 digits). To do so we first have to provide similar tools for the zeta function and its derivatives at integer points. These methods, and some extensions, are of independent value and are further pursued in this paper.

In Section 4 we record various reductions and interrelations of our MTW values (see Theorems 5, 6 and 7). In Section 5 we reprise two rigorous experiments [8] designed to use *integer relation methods* [16] to first explore the structure of the ensemble $\mathcal{D}_1$ and then to begin to study $\mathcal{D}$. Section 6 we present our new experimental work on the structure of $\mathcal{D}$. It also provides proofs of some experimentally discovered results. Finally, in Section 7 we make some summatory remarks.

2 Mordell–Tornheim–Witten ensembles

The multidimensional *Mordell–Tornheim–Witten (MTW) zeta function*

$$\omega(s_1,\ldots,s_{K+1}) \;:=\; \sum_{m_1,\ldots,m_K>0} \frac{1}{m_1^{s_1}\cdots m_K^{s_K}(m_1+\cdots+m_K)^{s_{K+1}}} \tag{1}$$

enjoys known relations [32], but remains mysterious with respect to many combinatorial phenomena, especially when we contemplate derivatives with respect to the s_i parameters. We shall refer to $K+1$ as the *depth* and $\sum_{j=1}^{k+1} s_j$ as the *weight* of ω.

A previous work [5] introduced and discussed a novel *generalized MTW zeta function* for positive integers M,N and nonnegative integers s_i,t_j—with constraints $M\geq N\geq 1$—together with a polylogarithm-integral representation:

$$\omega(s_1,\ldots,s_M \mid t_1,\ldots,t_N) := \sum_{\substack{m_1,\ldots,m_M,n_1,\ldots,n_N>0\\ \sum_{j=1}^M m_j=\sum_{k=1}^N n_k}} \prod_{j=1}^M \frac{1}{{m_j}^{s_j}} \prod_{k=1}^N \frac{1}{{n_k}^{t_k}} \tag{2}$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \prod_{j=1}^M \mathrm{Li}_{s_j}\left(e^{i\theta}\right) \prod_{k=1}^N \mathrm{Li}_{t_k}\left(e^{-i\theta}\right)\,\mathrm{d}\theta. \tag{3}$$

Here the *polylogarithm of order s* denotes $\mathrm{Li}_s(z) := \sum_{n\geq 1} z^n/n^s$ and its analytic extensions [31] and the (complex) number s is its *order*.

When some s-parameters are zero, there are convergence issues with this integral representation. One may, however, use principal-value calculus, or alternative representations given in [8] and expanded upon in Section 4.4.

When $N = 1$ the representation (3) devolves to the classic MTW form, in that

$$\omega(s_1, \ldots, s_{M+1}) = \omega(s_1, \ldots, s_M \mid s_{M+1}). \tag{4}$$

2.1 Generalized MTW sums

We also explore a wider *MTW ensemble* involving outer derivatives, introduced in [5], according to

$$\omega\left(\begin{array}{ccc} s_1, \ldots, s_M & | & t_1, \ldots, t_N \\ d_1, \ldots, d_M & | & e_1, \ldots e_N \end{array}\right) := \sum_{\substack{m_1,\ldots,m_M,n_1,\ldots,n_N>0 \\ \sum_{j=1}^M m_j = \sum_{k=1}^N n_k}} \prod_{j=1}^M \frac{(-\log m_j)^{d_j}}{{m_j}^{s_j}} \prod_{k=1}^N \frac{(-\log n_k)^{e_k}}{{n_k}^{t_k}} \tag{5}$$

$$= \frac{1}{2\pi} \int_0^{2\pi} \prod_{j=1}^M \mathrm{Li}_{s_j}^{(d_j)}\left(e^{i\theta}\right) \prod_{k=1}^N \mathrm{Li}_{t_k}^{(e_k)}\left(e^{-i\theta}\right) \mathrm{d}\theta, \tag{6}$$

where the s-th outer derivative of a polylogarithm is denoted $\mathrm{Li}_s^{(d)}(z) := \left(\frac{\partial}{\partial s}\right)^d \mathrm{Li}_s(z)$. Thus, the effective computation of (6) requires really robust and efficient methods for computing $\mathrm{Li}_s^{(d)}$ (Section 3.1.3 and sequela) and for high precision quadrature (Section 3.6).

We emphasize that all ω are real since we integrate over a full period; or more directly since the summand is real. Consistent with earlier usage, we now refer to $M + N$ as the *depth* and $\sum_{j=1}^M (s_j + d_j) + \sum_{k=1}^N (t_k + e_k)$ as the *weight* of ω.

To summarize, we study the MTW ensemble comprising the set

$$\mathcal{D} := \left\{\omega\left(\begin{array}{ccc} s_1, \ldots, s_M & | & t_1, \ldots, t_N \\ d_1, \ldots, d_M & | & e_1, \ldots e_N \end{array}\right) : s_i, d_i, t_j, e_j \geq 0;\ M \geq N \geq 1, M, N \in \mathbb{Z}^+\right\}. \tag{7}$$

3 Underlying special function and computational tools

To study ensemble $\mathcal{D}$ intensively, we must repeatedly differentiate polylogarithms with respect to their order, and be able to compute these and related functions, and the integrals (2) and (6) to very high precision (typically hundreds of digits or more).

The reason that such high precision is required stems from our applications of the PSLQ *integer relation algorithm* [11] in this research. Given an input vector of computed real numbers $(x_1, x_2, \cdots, x_n)$, PSLQ finds a nontrivial integer vector $(a_1, a_2, \cdots, a_n)$, if it exists, such that $a_1x_1 + a_2x_2 + \cdots a_nx_n = 0$. Such an algorithm is useful in this context because it often permits one to identify a high-precision computed numerical value in terms of an analytic formula involving certain well-known mathematical constants.

Suppose, for example, one conjectures an integral I is given as a sum of terms (with unknown rational coefficients), each of which is some known constant. Then by computing $x_1 = I$ and the terms $(x_i,\ 2 \leq i \leq n)$ to sufficiently high precision, and applying PSLQ to $(x_1, x_2, \cdots, x_n)$, the integer coefficients of such a relation (if it exists) can be found. Solving this relation for $x_1 = I$ produces a rational linear for I involving the conjectured constants. Even if PSLQ fails to find a numerically significant integer relation, it produces exclusion bounds within which no integer relation exists; often valuable information in this type of exploration.

For PSLQ (or any other relation-finding algorithm) to reliably recover a relation $(a_1, a_2, \cdots, a_n)$ of length n, where the coefficients (a_i) have maximum absolute value 10^d, requires at least dn-digit precision in the input vector, and at least dn-digit arithmetic in the operation of the algorithm.

3.1 Polylogarithms and their derivatives with respect to order

In regard to the needed polylogarithm values, [5] gives formulas such as below.

Proposition 1. *When $s = n$ is a positive integer,*

$$\mathrm{Li}_n(z) = \sum_{m=0}^{\infty}{}' \zeta(n-m)\frac{\log^m z}{m!} + \frac{\log^{n-1} z}{(n-1)!}\left(H_{n-1} - \log(-\log z)\right), \tag{8}$$

valid for $|\log z| < 2\pi$. Here $H_n := 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n}$, and the primed sum $\sum'$ means to avoid the singularity at $\zeta(1)$. For any complex order *s not a positive integer,*

$$\mathrm{Li}_s(z) = \sum_{m \geq 0} \zeta(s-m)\frac{\log^m z}{m!} + \Gamma(1-s)(-\log z)^{s-1}. \tag{9}$$

(This formula is valid for $s = 0$.)

In formula (8), the condition $|\log z| < 2\pi$ precludes its use when $|z| < e^{-2\pi} \approx 0.0018674$. For such small $|z|$, however, it typically suffices to use the definition

$$\mathrm{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s}. \tag{10}$$

Note that $\mathrm{Li}_0(z) = z/(1-z)$ and $\mathrm{Li}_1(z) = -\log(1-z)$.

In fact, we found that formula (10) is generally faster than (8) whenever $|z| < 1/4$, at least for precision levels in the range of 100 to 4000 digits.

3.1.1 Outer derivatives of general order polylogarithms

On carefully manipulating (9) for integer $k \geq 0$ we have for $|\log z| < 2\pi$ and $\tau \in [0, 1)$:

$$\mathrm{Li}_{k+1+\tau}(z) = \sum_{0 \leq n \neq k} \zeta(k+1+\tau-n)\frac{\log^n z}{n!} + \frac{\log^k z}{k!}\sum_{j=0}^{\infty} c_{k,j}(\mathcal{L})\,\tau^j, \tag{11}$$

see [27, §9, eqn. (51)]. Here $\mathcal{L} := \log(-\log z)$ and the c coefficients engage the *Stieltjes constants* γ_n, where $\gamma_0 = \gamma$ [27, §7.1], which occur in the asymptotic expansion

$$\zeta(z) = \frac{1}{z-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n}\gamma_n (z-1)^n.$$

Precisely

$$c_{k,j}(\mathcal{L}) = \frac{(-1)^j}{j!}\gamma_j - b_{k,j+1}(\mathcal{L}), \tag{12}$$

where the $b_{k,j}$ terms—corrected from [27, §7.1]—are given by

$$b_{k,j}(\mathcal{L}) := \sum_{\substack{p+t+q=j\\ p,t,q\geq 0}} \frac{\mathcal{L}^{\,p}}{p!}\frac{\Gamma^{(t)}(1)}{t!}(-1)^t f_{k,q}, \tag{13}$$

and $f_{k,q}$ is the coefficient of x^q in $\prod_{m=1}^{k}\frac{1}{1+x/m}$. This is calculable recursively via $f_{0,0}=1, f_{0,q}=0\ (q>0), f_{k,0}=1\ (k>0)$ and

$$f_{k,q} = \sum_{h=0}^{q}\frac{(-1)^h}{k^h}f_{k-1,q-h}. \tag{14}$$

Above we used the functional equation for the Γ function to remove singularities at negative integers.

While (11) has little directly to recommend it computationally, it is highly effective in determining derivative values with respect or order, as we shall see in (17).

Remark 1 (Harmonic numbers)**.** The next formula from [21] is helpful in organizing differentiation and highlights the relationship between the rising factorial or binomial coefficient and harmonic numbers: for $n \geq 1$

$$\frac{(-1)^\alpha}{\alpha!}\left(\frac{\mathrm{d}}{\mathrm{d}\lambda}\right)^\alpha \binom{\lambda}{n}\bigg|_{\lambda=0} = \frac{(-1)^n}{n}\,H_{n-1}^{[\alpha-1]}. \tag{15}$$

Herein, $\binom{\lambda}{n}$ denotes the binomial function $\Gamma(\lambda+1)/(\Gamma(n+1)\Gamma(\lambda-n+1))$, and we denote a *multiple harmonic number* by

$$H_{n-1}^{[\alpha]} := \sum_{n>i_1>i_2>\ldots>i_\alpha}\frac{1}{i_1 i_2\cdots i_\alpha}. \tag{16}$$

If $\alpha=0$ we set $H_{n-1}^{[0]} := 1$. We also recall that $H_{n-1}^{(\beta)} := \sum_{k<n} 1/k^\beta$ can be recovered for sums of products of $H_k^{[\alpha]}$. $\Diamond$

Then, $f_{k,1} = -H_k$ and $f_{k,2} = H_k^{[2]} = \frac{1}{2}H_k^2 + \frac{1}{2}H_k^{(2)}$, in terms of classical generalized harmonic numbers, while $c_{k,0} = H_k - \mathcal{L}$. With $k=\tau=0$ this yields (8).

To obtain the first derivative $\mathrm{Li}_{k+1}^{(1)}(z)$, we differentiate (11) at zero and so require the evaluation $c_{k,1}$. With $k=0$ and $j=1$ this supplies (25) below. More generally:

Theorem 1 (Derivatives for positive order)**.** *Fix $k=0,1,2\ldots$ and $m=1,2\ldots$. For $|\log z|<2\pi$ and $\mathcal{L}=\log(-\log z)$ one has*

$$\mathrm{Li}_{k+1}^{(m)}(z) = \sum_{0\leq n\neq k}\zeta^{(m)}(k+1-n)\frac{\log^n z}{n!} + m!\,c_{k,m}(\mathcal{L})\frac{\log^k z}{k!}. \tag{17}$$

Here, for $k \geq 1$, $c_{k,j}(\mathcal{L}) = \frac{(-1)^j}{j!}\gamma_j - b_{k,j+1}(\mathcal{L})$. (as in (13), (19) valid for $k = 0$) above

$$b_{k,m}(\mathcal{L}) := k \sum_{\substack{p+t+q=m \\ p,t,q\geq 0}} (-1)^t \frac{\mathcal{L}^p}{p!} \frac{\Gamma^{(t)}(1)}{t!} \frac{\beta^{(q)}(k,1)}{q!} = \sum_{\substack{p+t+q=j \\ p,t,q\geq 0}} \frac{\mathcal{L}^p}{p!} \frac{\Gamma^{(t)}(1)}{t!} (-1)^t f_{k,q}, \tag{18}$$

where $\beta^{(q)}(k,1)$ is the q-th derivative of the beta function $\beta(k,x)$ wrt x at 1, the f coefficients are given recursively by $f_{0,0} = 1, f_{0,q} = 0$ $(q > 0), f_{k,0} = 1$ $(k > 0)$ while

$$f_{k,q} = \sum_{h=0}^{q} \frac{(-1)^h}{k^h} f_{k-1,q-h}. \tag{19}$$

Note that symmetric divided differences allow one to rapidly check (17) to moderate precision (say 50 digits). For $k = -1$, or, in other words, for $\mathrm{Li}_0^{(m)}(z)$, things are simpler, as we may use (9):

Theorem 2 (Derivatives for zero order)**.** *With $\Gamma^{(t)}(1)$ and $\mathcal{L} = \log(-\log z)$ as above for arbitrary z, we have for m any positive integer*

$$\mathrm{Li}_0^{(m)}(z) = \sum_{n\geq 0} \zeta^{(m)}(-n) \frac{\log^n z}{n!} - \sum_{t=0}^{m} (-1)^t \binom{m}{t} \Gamma^{(t)}(1) \frac{\mathcal{L}^{m-t}}{\log z}. \tag{20}$$

Below we give an effective algorithm for $\Gamma^{(t)}(1)$ in (39). We also provide the necessary tools for computation of $\zeta^{(m)}(-n)$ as required in (17) and (20).

3.1.2 Another potential method

An alternative way to calculate derivatives of polylogarithms avoids recourse to ζ or η derivatives, the tradeoff being that one needs a side-quadrature calculation (albeit one involving only an elementary integrand). P. Jodrá observes (`http://rspa.royalsocietypublishing.org/content/464/2099/3081.full`) that polylogarithms can be written

$$\mathrm{Li}_s(z) \;=\; \frac{z}{\Gamma(s+1)} \int_0^1 \frac{(-\log u)^s}{(1-zu)^2}\, du.$$

Multiplying through by $\Gamma(s+1) =: s!$, one has convenient recursion for the d-th derivative:

$$\mathrm{Li}_s^{(d)}(z) = -\frac{1}{s!} \sum_{j=0}^{d-1} \binom{d}{j} \Gamma^{(d-j)}(s+1) \mathrm{Li}_s^{(j)}(z) + \frac{1}{s!}\, I_{s,d}(z), \tag{21}$$

where

$$I_{s,d}(z) := z \int_0^1 \log^d(-\log u) \frac{(-\log u)^s}{(1-zu)^2}\, du. \tag{22}$$

The Γ=derivatives here are again fundamental. The idea, then is to build a table of $\mathrm{Li}_s^{(d)}$ using this recursion, with a log log-log integral required—but only once—for every new derivative. In this way, for each abscissa z in an overall MTW quadrature, a chain of derivatives can be calculated and stored. Moreover, changing variables ($x = -\log u$) and using the binomial theorem leads to

$$I_{s,d}(z) = z\ \Gamma^{(d)}(s+1) + \sum_{n=2}^{\infty} \left(\sum_{k=0}^{d} \binom{d}{k} (-\log n)^k\ \Gamma^{(d-k)}(s+1) \right) \frac{z^n}{n^s}. \tag{23}$$

Hence, we opt to use the left side of (23), as the right includes calculating the series we wish to avoid summing. That said, (23) leads to a quick verification of (21) and (22).

3.1.3 The special case $s = 1$ and $z = e^{i\theta}$

Most importantly, in light of integral (6) we may write, for $0 < \theta < 2\pi$,

$$\mathrm{Li}_1(e^{i\theta}) = -\log\left(2\sin\left(\frac{\theta}{2}\right)\right) + \frac{(\pi-\theta)}{2} i. \tag{24}$$

As described , the order-derivatives $\mathrm{Li}_s'(z) = \mathrm{d}(\mathrm{Li}_s(z))/\,\mathrm{d}s$ for integer s, can be computed via

$$L_1'(z) = \sum_{n=1}^{\infty} \zeta'\,(1-n)\,\frac{\log^n z}{n!} - \gamma_1 - \frac{1}{12}\,\pi^2 - \frac{1}{2}\,(\gamma + \log(-\log z))^2\,, \tag{25}$$

which, as before, is valid whenever $|\log z| < 2\pi$. Here γ_1 is the *second Stieltjes constant* [3, 27]. For small $|z|$, it again suffices to use the elementary form

$$\mathrm{Li}_s'(z) = -\sum_{n=1}^{\infty} \frac{z^k \log k}{k^s}. \tag{26}$$

Relation (25) can be applied to yield the formula

$$\mathrm{Li}_1'(e^{i\theta}) = \sum_{n=1}^{\infty} \zeta'\,(1-n)\,\frac{(i\theta)^n}{n!} - \gamma_1 - \frac{1}{12}\,\pi^2 - \frac{1}{2}\,(\gamma + \log(-i\theta))^2\,, \tag{27}$$

valid and convergent for $|\theta| < 2\pi$.

Given such formulas, to evaluate MTW values one may use pure quadrature, a convergent series, or a combination of quadrature and series. All of these are exploited in the MTW examples of [27].

3.2 Values of ζ at integer arguments

Effective use of (8,9) requires precomputed values of the zeta function and its derivatives at integer arguments (see [3, 25]).

3.2.1 Values of ζ at positive even integer arguments

As we shall require $\zeta(n)$ for many integers, the following approach, used in [9], is efficient. First, to compute $\zeta(2n)$, observe that

$$\begin{aligned}\coth(\pi x) &= \frac{-2}{\pi x} \sum_{k=0}^{\infty} \zeta(2k)(-1)^k x^{2k} \ = \ \cosh(\pi x)/\sinh(\pi x) \\ &= \frac{1}{\pi x} \cdot \frac{1 + (\pi x)^2/2! + (\pi x)^4/4! + (\pi x)^6/6! + \cdots}{1 + (\pi x)^2/3! + (\pi x)^4/5! + (\pi x)^6/7! + \cdots}.\end{aligned} \tag{28}$$

Let $P(x)$ and $Q(x)$ be the numerator and denominator polynomials obtained by truncating these series to n terms. The approximate reciprocal $R(x)$ of $Q(x)$ can be gotten from the Newton iteration

$$R_{k+1}(x) := R_k(x) + [1 - Q(x) \cdot R_k(x)] \cdot R_k(x), \tag{29}$$

where the degree of the polynomial and numeric precision of the coefficients are dynamically increased, approximately doubling when convergence has been achieved—at a given degree and precision—until the final desired degree and precision are achieved. When complete, the quotient P/Q is the product $P(x) \cdot R(x)$. Desired $\zeta(2k)$ values can then be obtained from coefficients of this product polynomial as in [9]. Recall that $\zeta(0) = -1/2$.

The *Bernoulli numbers* B_{2k} are also needed. They now can be obtained from [33, Eqn. (25.6.2)]

$$B_{2k} = (-1)^{k+1} \frac{2(2k)!\zeta(2k)}{(2\pi)^{2k}}. \tag{30}$$

3.2.2 Values of ζ at positive odd integer arguments

Positive odd zeta values can be efficiently found via two Ramanujan-style formulas: [9, 18]:

$$\zeta(4N+3) = -2\sum_{k=1}^{\infty} \frac{1}{k^{4N+3}(\exp(2k\pi) - 1)} - \pi(2\pi)^{4N+2} \sum_{k=0}^{2N+2} (-1)^k \frac{B_{2k}B_{4N+4-2k}}{(2k)!(4N+4-2k)!}, \tag{31}$$

$$\zeta(4N+1) = -\frac{1}{N}\sum_{k=1}^{\infty} \frac{(2\pi k + 2N)\exp(2\pi k) - 2N}{k^{4N+1}(\exp(2k\pi) - 1)^2} - \frac{\pi(2\pi)^{4N}}{2N} \sum_{k=1}^{2N+1} (-1)^k \frac{B_{2k}B_{4N+2-2k}}{(2k-1)!(4N+2-2k)!}.$$

3.2.3 Values of ζ at negative integer arguments

Finally, zeta can be evaluated at negative integers by the following formulas [33, (25.6.3), (25.6.4)]:

$$\zeta(-2n+1) = -\frac{B_{2n}}{2n} \qquad \text{and} \qquad \zeta(-2n) = 0. \tag{32}$$

3.3 Derivatives of ζ at integer arguments

Precomputed zeta-derivative values are prerequisite for the efficient use of formulas we have presented so far, including the crucial formulas (17), (20), (25) and (27).

3.3.1 Derivatives of ζ at positive integer arguments

Remark 2 (Using Computer Algebra Systems)**.** For the simplest instances of the just-mentioned formulas, built-in zeta derivative facilities of *Maple* or *Mathematica* suffice; but from our experience this approach is not robust. For example, *Maple 16* produces 2000 digits of quantities such as $\zeta^{(10}(2)$ quite rapidly, and 5000-digit results in roughly 100 seconds. Yet while *Mathematica* 9 verifies the 2000-digit results in cases we tried (more slowly), it fails at 5000-digit precision. Also, *Mathematica* 9 inexplicably refuses to compute $\zeta^{(4)}(0)$ at all; similarly for higher derivatives at zero. $\diamondsuit$

For positive integers, derivatives of the zeta function can be computed via a series-accelerated algorithm for derivatives of the *Dirichlet eta function* (or alternating zeta function), given as

$$\eta(s) := \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^s} = (1 - 2^{1-s})\zeta(s). \tag{33}$$

For practical computation of eta or its derivatives, any of several alternating series acceleration schemes can be used. The corresponding values of zeta derivatives can then be found by solving (33) for $\zeta(s)$ and then taking formal derivatives, for example

$$\zeta'(s) = \frac{\eta'(s)}{(1 - 2^{1-s})} - \frac{2^{1-s}\eta(s)\log 2}{(1 - 2^{1-s})^2}. \tag{34}$$

Example 1 (Alternating series acceleration [27, 26]). This is illustrated in the following *Mathematica* code (for argument ss, and precision prec digits):

```
zetaprime[ss_] :=
 Module[{s, n, d, a, b, c}, n = Floor[1.5*prec]; d = (3 + Sqrt[8])^n;
   d = 1/2*(d + 1/d);
  {b, c, s} = {-1, -d, 0};
  Do[c = b - c;
   a = 1/(k + 1)^ss *(-Log[k + 1]);
   s = s + c*a;
   b = (k + n)*(k - n)*b/((k + 1)*(k + 1/2)), {k, 0, n - 1}];
  (s/d - 2^(1 - ss)*Log[2]*Zeta[ss])/(1 - 2^(1 - ss))]
```

In this algorithm, that logarithm and zeta values can be precalculated, and so do not significantly add to run time. A similar approach works well for higher derivatives of zeta, although the resulting generalization of (34) becomes progressively more complicated. ◊

3.3.2 First derivative of of ζ at zero and negative integer arguments

The functional equation $\zeta(s) = 2(2\pi)^{s-1} \sin \frac{\pi s}{2} \; \Gamma(1-s)\,\zeta(1-s)$ lets one extract $\zeta'(0) = -(\log 2\pi)/2$ and for even $m = 2, 4, 6, \ldots$

$$\zeta'(-m) := \frac{d}{ds}\zeta(s)|_{s=-m} = \frac{(-1)^{m/2} m!}{2^{m+1}\pi^m}\,\zeta(m+1) \tag{35}$$

[27, p. 15], while for odd $m = 1, 3, 5 \ldots$ on the other hand,

$$\zeta'(-m) = \zeta(-m)\left(\gamma + \log 2\pi - H_m - \frac{\zeta'(m+1)}{\zeta(m+1)}\right). \tag{36}$$

We now delineate methods more suited to higher derivatives at negative integers.

3.4 Higher derivatives of ζ at negative integers

To approach these values we again need recourse to the gamma function.

3.4.1 Derivatives of Γ at positive integers

(a) Let $g_n := \Gamma^{(n)}(1)$. Now it is well known [33, (5.7.1) and (5.7.2)] that

$$\Gamma(z+1)\,\mathcal{C}(z) = z\,\Gamma(z)\,\mathcal{C}(z) = z \tag{37}$$

where $\mathcal{C}(z) := \sum_{k=1}^{\infty} c_k z^k$ with $c_0 = 0, c_1 = 1, c_2 = \gamma$ and

$$(k-1)c_k = \gamma c_{k-1} - \zeta(2)\,c_{k-2} + \zeta(3)\,c_{k-3} - \cdots + (-1)^k\,\zeta(k-1)\,c_1, \tag{38}$$

Thus, differentiating (37) by Leibnitz' formula, for $n \ge 1$ we have

$$g_n = -\sum_{k=0}^{n-1} \frac{n!}{k!}\,g_k\,c_{n+1-k}. \tag{39}$$

(b) More generally, for positive integer m we have

$$\Gamma(z+m)\;\mathcal{C}(z) = (z)_m \tag{40}$$

where $(z)_m := z(z+1)\cdots(z+m-1)$ is the *rising factorial*. Whence, letting $g_n(m) := \Gamma^{(n)}(m)$ so that $g_n(1) = g_n$, we may apply the product rule to (40) and obtain

$$g_n(m) = -\sum_{k=0}^{n-1} \frac{n!}{k!}\,g_k(m)\,c_{n+1-k} + \frac{D_m^{n+1}}{n+1}. \tag{41}$$

Here D_m^n is the n-th derivative of $(x)_m$ evaluated at $x=0$; zero for $n > m$. For $n \le m$ values are easily obtained symbolically or in terms of *Stirling numbers of the first kind*:

$$D_m^n = \sum_{k=0}^{m-n} s\,(m,k+n)\,(k+1)_n\,(m-1)^k = (n+1)!\,(-1)^{m+n+1} s\,(m,1+n)\,. \tag{42}$$

Thus, $\frac{D_m^n}{(n+1)} = n!|s(m,1+n)|$ and so for $n,m>1$ we obtain the recursion

$$\frac{g_n(m)}{n!} = -\sum_{k=0}^{n-1} \frac{g_k(m)}{k!}\,c_{n+1-k} + |s(m,1+n)|. \tag{43}$$

where for integer $n,k \ge 0$

$$s(n,k) = s(n-1,k-1) - (n-1)\,s(n-1,k)\,, \tag{44}$$

as in [33, Equation (26.8.18)].

3.4.2 Apostol's formulas for $\zeta^{(k)}(m)$ at negative integers

For $n = 1,2,\ldots$, with $\kappa := -\log(2\pi) - \frac{1}{2}\pi i$, we have Apostol's formulas [33, (25.6.13) and (25.6.14)]:

$$(-1)^k \zeta^{(k)}(1-2n) = \frac{2(-1)^n}{(2\pi)^{2n}} \sum_{m=0}^{k}\sum_{r=0}^{m} \binom{k}{m}\binom{m}{r} \mathrm{Re}(\kappa^{k-m})\,\Gamma^{(r)}(2n)\,\zeta^{(m-r)}(2n)\,, \tag{45}$$

$$(-1)^k \zeta^{(k)}(-2n) = \frac{2(-1)^n}{(2\pi)^{2n+1}} \sum_{m=0}^{k}\sum_{r=0}^{m} \binom{k}{m}\binom{m}{r} \mathrm{Im}(\kappa^{k-m})\,\Gamma^{(r)}(2n+1)\,\zeta^{(m-r)}(2n+1)\,. \tag{46}$$

Since in (41) only initial conditions rely on m, equations (45) and (46) are well fitted to work with (41) (along with (44), and (38)). The derivatives $\zeta^{(m)}(0)$ needed in (45) can be computed by either the methods of [3, Thm. 3] or [25, §5(c)]. Indeed

Theorem 3 (Apostol)**.** *If $z = -\log(2\pi) - i\pi/2$ and $n \geq 0$, we have*

$$(-1)^n \frac{\zeta^{(n)}(0)}{n!} = \frac{1}{\pi} \frac{\operatorname{Im}(z^{n+1})}{(n+1)!} + \frac{1}{\pi} \sum_{k=1}^{n-1} a_k \frac{\operatorname{Im}(z^{n-k})}{(n-k)!} \tag{47}$$

where the coefficients a_k are determine by the Laurent expansion

$$\Gamma(s)\zeta(s) = \frac{1}{s-1} + \sum_{n=0}^{\infty} a_n (s-1)^n, \tag{48}$$

so that $a_n = c_{n+1} + \sum_{k=0}^{n} c_{n-k}\gamma_k$ where $c_n = \Gamma^n(1)/n! = g_n/n!$ is computable as in (39).

3.5 More general character L-series

We make a brief detour to general real L-series, see [20], given by

$$\mathrm{L}_{\pm d}(s) := \sum_{n>0} \frac{\chi_{\pm d}(n)}{n^s} = \frac{1}{d^s} \sum_{k=1}^{d-1} \binom{\pm d}{k} \zeta\left(s, \frac{k}{d}\right). \tag{49}$$

For $d \geq 3$ we use the multiplicative characters $\chi_{\pm d}(n) := \binom{\pm d}{n}$ in terms of the generalized *Legendre-Jacobi symbol* and for later use we set $\chi_1(n) := 1, \chi_{-2}(n) := (-1)^n$. Then $\mathrm{L}_1 := \zeta, \mathrm{L}_{-2} := \eta$, the alternating zeta function.

Remark 3 (Primitive series)**.** Each such L-series, when *primitive* [20, p. 158] and [2, 17], obeys a simple functional equation:

$$\mathrm{L}_{\pm d}(s) = C(s) \left\{ \begin{array}{c} \sin(s\pi/2) \\ \cos(s\pi/2) \end{array} \right\} \mathrm{L}_{\pm d}(1-s), \qquad C(s) := 2^s \pi^{s-1} d^{-s+1/2} \Gamma(1-s) \tag{50}$$

and can be summed at integer values:

$$\begin{aligned} \mathrm{L}_{\pm d}(1-2m) &= \left\{ \begin{array}{l} (-1)^m R (2m-1)!/(2d)^{2m-1} \\ 0 \end{array} \right. \\ \mathrm{L}_{\pm d}(-2m) &= \left\{ \begin{array}{l} 0 \\ (-1)^m R' (2m)!/(2d)^{2m} \end{array} \right. \\ \mathrm{L}_{+d}(2m) &= R d^{-1/2} \pi^{2m}, \qquad \mathrm{L}_{-d}(2m-1) = R' d^{-1/2} \pi^{2m-1}, \end{aligned} \tag{51}$$

where m is a positive integer and R, R' are rational numbers which depend on m, d. For $d = 1$ these engage the Bernoulli numbers while for $d = -4$ the Euler numbers appear. $\diamondsuit$

Remark 4 (Lerch's formula)**.** The following parametric version of (9) holds:

$$\sum_{n=0}^{\infty} \frac{z^{(n+\nu)}}{(n+\nu)^s} = \Gamma(1-s)(-\log z)^{s-1} + \sum_{r=0}^{\infty} \zeta(s-r, \nu) \frac{(\log z)^r}{r!}. \tag{52}$$

Here $\zeta(s,\nu)$ is the *Hurwitz zeta* function, $s \neq 1,2,3,\ldots$, $\nu \neq 0.-1,-2,\ldots$, and as before $|\log z| < 2\pi$, see [28, Vol 1, p.29, eqn. (8)]. Then (9) is the case $\nu = 1$. Using (52) it is possible to substantially extend (17). We obtain

$$\sum_{n=0}^{\infty} \frac{z^{(dn+k+\varepsilon)}}{(dn+k+\varepsilon)^s} = \frac{1}{d}\Gamma(1-s)(-\log z)^{s-1} + \sum_{r=0}^{\infty} \zeta\left(s-r, \frac{k+\varepsilon}{d}\right) \frac{d^{r-s}(\log z)^r}{r!}. \tag{53}$$

From this we obtain for $k = 1,2,\ldots,d-1$, $s \neq 1,2,3,\ldots$, and $0 < \varepsilon < 1$ that

$$\sum_{n=1}^{\infty} \binom{\pm d}{n} \frac{z^{(n+\varepsilon)}}{(n+\varepsilon)^s} = \sum_{r=0}^{\infty} \left(\frac{1}{d^{s-r}} \sum_{k=1}^{d-1} \binom{\pm d}{k} \zeta\left(s-r, \frac{k+\varepsilon}{d}\right)\right) \frac{(\log z)^r}{r!}, \tag{54}$$

since $\sum_{m=1}^{d} \binom{\pm d}{m} = 0$ for $d > 2$. $\Diamond$

We now have a tractable formula for differentiation wrt the order. First, for primitive $\pm d$ define

$$\mathrm{L}_{\pm d}(s;z) := \sum_{n=1}^{\infty} \binom{\pm d}{n} \frac{z^n}{n^s} \tag{55}$$

$$\mathrm{L}_{\pm d}^{(m)}(s;z) := \frac{\partial^m}{\partial s^m} \mathrm{L}_{\pm d}(s;z). \tag{56}$$

Then for $m = 0,1,2,\ldots$, we can write

$$\begin{aligned}\mathrm{L}_{\pm d}^{(m)}(s;z) &:= \sum_{n=1}^{\infty} \binom{\pm d}{n} \frac{(\log n)^m}{n^s} z^n \\ &= \sum_{r=0}^{\infty} \frac{\partial^m}{\partial s^m} \left(\frac{1}{d^{s-r}} \sum_{k=1}^{d-1} \binom{\pm d}{k} \zeta\left(s-r, \frac{k}{d}\right)\right) \frac{(\log z)^r}{r!}\end{aligned} \tag{57}$$

We can now derive the character counterpart to (17) namely:

Theorem 4 (Primitive L-series)**.** *For $d = 3,4,\ldots$ and all s (since the poles at $s = 1$ cancel) we have*

$$\mathrm{L}_{\pm d}^{(m)}(s;z) = \sum_{r=0}^{\infty} \mathrm{L}_{\pm d}^{(m)}(s-r) \frac{(\log z)^r}{r!} \tag{58}$$

when $|\log z| < 2\pi$.

We are left with the job of generalizing (45) and (46), from ζ to more general L-series. This can be achieved from the requisite functional equation in (50) by the methods of [3]. The details and related extensions form the basis of [6].

3.5.1 L-series derivatives at negative integers

We begin for $d = 1,2,\ldots,$ with (50) which we rewrite as

$$\sqrt{d}\,\mathrm{L}_{\pm d}(1-s) = \Psi_{\pm d}(s)\,\mathrm{L}_{\pm d}(s), \qquad \Psi_{\pm d}(s) := \left(\frac{d}{2\pi}\right)^s \left\{ \begin{array}{c} 2\,\mathrm{Re}\, e^{i\pi s/2} \\ 2\,\mathrm{Im}\, e^{i\pi s/2} \end{array} \right\} \Gamma(s). \tag{59}$$

Then for real s and $\kappa_d := \log(d/(2\pi)) - i\pi/2$:

$$\sqrt{d}\,\mathrm{L}_{+d}(1-s) = \mathrm{Re}\; 2e^{s\kappa_d}\,\Gamma(s)\,\mathrm{L}_{+d}(s), \tag{60}$$

$$\sqrt{d}\,\mathrm{L}_{-d}(1-s) = \mathrm{Im}\; 2e^{s\kappa_d}\,\Gamma(s)\,\mathrm{L}_{-d}(s). \tag{61}$$

Two applications of Leibnitz' formula for n-fold differentiation wrt s leads to explicit analogues of (45) and (46). For all except the principle character, this is also applicable at $s = 0$.

When s is a positive integer things again simplify. As with ζ more work is needed for L-series derivatives at zero. It helps to know $\zeta(0,a) = 1/2 - a, \zeta'(0,a) = \log\Gamma(a) - \frac{1}{2}\log(2\pi)$.

3.5.2 Character MTW sums

On this foundation, one may then analyse extended MTW sums in which more general character polylogarithms replace the classical one in (6). That is, we may consider

$$\mu_{d_1,d_2}(q,r,s) := \sum_{n,m>0} \frac{\chi_{d_1(m)}}{m^q}\frac{\chi_{d_2(n)}}{n^r}\frac{1}{(m+n)^s} \tag{62}$$

$$= \frac{1}{\Gamma(s)}\int_0^1 \mathrm{L}_{d_1}(q;x)\,\mathrm{L}_{d_2}(r;x)(-\log x)^{s-1}\,\frac{\mathrm{d}x}{x} \tag{63}$$

where as before for $d > 2$, $\chi_d(n) := \binom{d}{n}$, and $\chi_{-2}(n) := (-1)^n$.

We may now also take derivatives in (63). Theorem 5 below extends to show that each $\mu_{d_1,d_2}(q,r,s)$ is a superposition of pure character Euler sums. Polylogarithms and Euler sums based primarily on mixes of χ_{-4} and χ_1 are studied at length in [22].

3.6 Tanh-sinh quadrature

Efficient quadrature computation is needed in both (2) and (6). Since these integrands are often badly behaved at endpoints, we recommend *tanh-sinh quadrature*, which is remarkably insensitive to singularities at endpoints of the interval of integration. Tanh-sinh quadrature also has a distinct advantage over methods such as Gaussian quadrature (only applicable for functions that are regular at endpoints), since the cost of computing abscissas and weights increases only linearly with N (the number of integration points) in tanh-sinh quadrature, whereas this cost increases quadratically with N in Gaussian quadrature.

Tanh-sinh quadrature approximates the integral of $f(x)$ on $(-1,1)$ as

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} f(g(t))g'(t)\,\mathrm{d}t \;\approx\; h\sum_{j=-N}^{N} w_j f(x_j), \tag{64}$$

for given $h > 0$, where abscissas x_j and weights w_j are given by

$$\begin{aligned} x_j = g(hj) \;&=\; \tanh\left(\pi/2\cdot\sinh(hj)\right) \\ w_j = g'(hj) \;&=\; \pi/2\cdot\cosh(hj)/\cosh\left(\pi/2\cdot\sinh(hj)\right)^2. \end{aligned} \tag{65}$$

Here N is chosen so that terms of the summation beyond N are smaller in absolute value than the "epsilon" of numeric precision used. Abscissas x_j and weights w_j can be precomputed, and then applied to all quadrature calculations. For many integrands, including those in (2) and (6), reducing h by half in (64) and (65) roughly doubles the number of correct digits, provided calculations are done to a precision level at least that desired for the final result. Full details are given in [13].

Remark 5. It suffices to integrate the real part of the integrand in (2) and (6) from 0 to π, and divide by π. Also, when computing $\mathcal{D}$ values for many m, n, p and q, it is much faster to precompute polylog derivative functions (sans exponents) at each tanh-sinh abscissa point x_j. Thence, during quadrature, each function evaluation in (6) consists of table look-ups and a few multiplications. In our tests, this change alone accelerated the quadrature calculations by a factor of over 1000. $\diamondsuit$

4 More subtle MTW interrelations

We now return to our objects of central interest.

4.1 Reduction of classical MTW values and derivatives

Partial fraction manipulations allow one to relate partial derivatives of MTWs. Such a relation in the classical three parameter setting is:

Theorem 5 (Reduction of classical MTW derivatives [5])**.** *Let nonnegative integers a, b, c and r, s, t be given. Set $N := r + s + t$. Define the shorthand notation*

$$\omega_{a,b,c}(r, s, t) := \omega \left(\begin{array}{cc|c} r\ , & s & t \\ a\ , & b & c \end{array} \right).$$

Then for $\delta := \omega_{a,b,c}$ we have

$$\delta(r, s, t) = \sum_{i=1}^{r} \binom{r+s-i-1}{s-1} \delta\left(i, 0, N-i\right) + \sum_{i=1}^{s} \binom{r+s-i-1}{r-1} \delta\left(0, i, N-i\right). \tag{66}$$

In the case that $\delta = \omega$ this shows that each classical MTW value is a finite positive integer combination of multi zeta values (MZVs) as discussed below. Of course, (66) holds for any δ satisfying the recursion (without being restricted to partial derivatives).

Remark 6. (Computing and validating ω constants). For fixed partial derivatives a, b, c set $\delta(r, s, t) := \omega_{a,b,c}(r, s, t)$. As exploited in [8], we have

$$\delta(r, s, t-1) = \delta(r-1, s, t) + \delta(r, s-1, t). \tag{67}$$

Correspondingly $\delta(q, r, s, t) := \omega_{a,b,c,d}(q, r, s, t)$ satisfies the recurrence

$$\delta\left(q, r, s, t\right) = \delta\left(q-1, r, s, t+1\right) + \delta\left(q, r-1, s, t+1\right) + \delta\left(r, s-1, t+1\right). \tag{68}$$

Then agreement with (67) or (68) gives one significant assurance that the computation of (6) is correct. Moreover, for larger values of r, s, t the double sum $\delta(r, s, t)$ may be computed quickly to fair accuracy directly from the definition (5). $\diamondsuit$

We reproduce some evaluations from our previous study (in some cases extended to more digits):

Example 2.

$$\omega_{1,1,0}(1,0,3) = 0.07233828360935031113948057244763953352659776102642063 95\ldots \quad (69)$$

$$\omega_{1,1,0}(2,0,2) = 0.29482179736664239559157187114891977101838854886937848 12\ldots \quad (70)$$

$$\omega_{1,1,0}(1,1,2) = 0.14467656721870062227896114489527906705319552205284127 90\ldots \quad (71)$$

$$\omega_{1,0,1}(1,0,3) = 0.14042163138773371925054281123123563768136197000104827 66\ldots \quad (72)$$

$$\omega_{1,0,1}(2,0,2) = 0.40696928390140268694035563517591371639834128770661373 81\ldots \quad (73)$$

$$\omega_{1,0,1}(1,1,2) = 0.43097253394888316942248176511038963971077201581912157 52\ldots \quad (74)$$

$$\omega_{0,1,1}(2,1,1) = 3.00297121355668005079211509351534225995879828374320045 98\ldots \quad (75)$$

Based on these numerical values, we note that $\omega_{1,1,0}(1,1,2) = 2\,\omega_{1,1,0}(1,0,3)$, and

$$\begin{aligned}
&\omega_{1,0,1}(1,0,3) + \omega_{1,0,1}(0,1,3) - \omega_{1,0,1}(1,1,2)\\
&\quad = \; 0.14042163138773371924 7\ldots + 0.29055090256114945012\ldots - 0.43097253394888316942\ldots\\
&\quad = \; 0.00000000000000000000\ldots,
\end{aligned}$$

both in accord with Theorem 5. A PSLQ run on the above data predicts that

$$\zeta''(4) \stackrel{?}{=} 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2) - 2\,\omega_{1,0,1}(2,0,2), \quad (76)$$

which discovery, proven in [8], also validated the effectiveness of our high-precision techniques. This identity is formally distinct from the corresponding case of (90) below. $\diamondsuit$

4.2 Relations when $M \geq N \geq 2$

Since $\sum t_k = \sum s_j$, we deduce from (2), by a partial fraction argument that

Theorem 6 (Relations for general ω)**.**

$$\begin{aligned}
&\sum_{k=1}^{N} \omega\left(\begin{array}{c|c} s_1,\ldots,s_M & t_1,\ldots,t_{k-1},t_k-1,t_{k+1},\ldots,t_N \\ d_1,\ldots,d_M & e_1,\ldots e_N \end{array}\right)\\
&= \sum_{j=1}^{M} \omega\left(\begin{array}{c|c} s_1,\ldots,s_{j-1},s_j-1,s_{j+1},\ldots,s_M & t_1,\ldots,t_N \\ d_1,\ldots,d_M & e_1,\ldots e_N \end{array}\right). \quad (77)
\end{aligned}$$

For $N > 1$ we thus find relations but have found no full reduction.

4.3 Complete reduction of MTW values when $N = 1$

For $N = 1$ and general M there is a result like Theorem 5, and Theorem 6 implies every MTW value (without any derivatives) is a finite sum of MZV's. The basic tool is the partial fraction

$$\frac{m_1+m_2+\ldots+m_k}{m_1^{a_1}m_1^{a_2}\cdots m_k^{a_k}} = \frac{1}{m_1^{a_1-1}m_1^{a_2}\cdots m_k^{a_k}} + \frac{1}{m_1^{a_1}m_1^{a_2-1}\cdots m_k^{a_k}} + \frac{1}{m_1^{a_1}m_1^{a_2}\cdots m_k^{a_k-1}}.$$

We arrive at:

Theorem 7 (Complete reduction of $\omega(a_1, a_2, \ldots, a_M \mid b)$ [8]). *For nonnegative values of $a_1, a_2, \ldots, a_M, b$ the following holds:*

a) Each $\omega(a_1, a_2, \ldots, a_M \mid b)$ is a finite sum of values of MZVs of depth M and weight $a_1 + a_2 + \cdots + a_M + b$.

b) In particular, if the weight is even and the depth odd or the weight is odd and the depth is even then the sum reduces to a superposition of sums of products of that weight of lower weight MZVs.

4.4 Degenerate MTW derivatives with zero numerator values

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In Theorem 7 we included no derivative values—a zero value may still have a log term in the corresponding variable and thus obstruct depth reduction—nor have we included $M \geq N \geq 2$. For example, it appears unlikely that

$$\omega\left(\begin{array}{cc|c} 1\ , & 0 & 2 \\ 0\ , & 1 & 0 \end{array}\right) = \sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^{n-1} \frac{\log(n-m)}{m} \tag{78}$$

is reducible to derivatives of MZVs. Likewise, for $s > 2$ we have

$$\omega\left(\begin{array}{cc|c} 0\ , & 0 & s \\ 0\ , & 1 & 0 \end{array}\right) = -\sum_{n=2}^{\infty} \frac{\log \Gamma(n)}{n^s}. \tag{79}$$

We observe that such ω values with terms of order zero cannot be computed directly from the integral form of (6) without special attention to convergence at the singularities.

Example 3. Though it is unlikely that MTW derivatives are finite superpositions of MZV derivatives, it is possible to establish (non-finitary) relations. Consider

$$\begin{aligned}
\omega\left(\begin{array}{cc|c} r\ , & 0 & s \\ 0\ , & 1 & 0 \end{array}\right) &= -\sum_{m,n\geq 1} \frac{1}{m^r} \log n \frac{1}{(m+n)^s} \qquad (80) \\
&= -\sum_{N \geq 1} \frac{1}{N^s} \sum_{M=1}^{N-1} \frac{\log(N-M)}{M^r} \\
&= \zeta_{1,0}(s,r) + \sum_{k\geq 1} \frac{1}{k} \zeta(s+k, r-k).
\end{aligned}$$

Here, $\zeta_{1,0}(s,r)$ is the first parametric derivative $\partial\zeta(s,r)/\partial s$. What is unsatisfactory about this expression is that the k-sum is not a finite superposition—though it *does* converge. $\Diamond$

4.4.1 Computation of ω in degenerate cases

Recall again that integral form (6) is used freely only when all s_j, t_k numerator (non-logarithmic) parameters are non-zero; so we must attend to such degenerate cases. for which one can use formulas like:

$$\omega_{a,b,c}(q,r,s) = \omega\left(\begin{array}{cc|c} q\ ,\ r & & s \\ a\ ,\ b & & c \end{array}\right) = \int_0^\infty \left(\frac{x^{s-1}}{\Gamma(s)}\right)^{(c)} \mathrm{Li}_q^{(a)}(e^{-x})\,\mathrm{Li}_r^{(b)}(e^{-x})\,\mathrm{d}x, \tag{81}$$

which is valid when $q \geq 0, r \geq 0, s > 0$, with $q + r + s > 2$, and $a \geq 0, b \geq 0, c \geq 0$. Here the notation $(\cdot)^{(c)}$ denotes the c-th partial derivative of the expression in parentheses with respect to s. This may be seen by expanding the integrand and using

$$\frac{1}{\Gamma(s)}\int_0^\infty \mathrm{e}^{-wx} x^{s-1} dx = \frac{1}{w^s},$$

for $s, w > 0$. To apply the tanh-sinh quadrature rule to evaluate (81), it is necessary to convert it to a finite interval. This can be remedied by breaking the integral into two parts (0 to 1, and 1 to ∞), and then using the substitution $u = e^{-x}$ for the second integral:

$$\begin{aligned}\omega_{a,b,c}(q,r,s) = &\int_0^1 \left(\frac{x^{s-1}}{\Gamma(s)}\right)^{(c)} \mathrm{Li}_q^{(a)}(e^{-x})\,\mathrm{Li}_r^{(b)}(e^{-x})\,\mathrm{d}x \\ &+ \int_0^{1/e} \left(\frac{(-\log u)^{s-1}}{\Gamma(s)}\right)^{(c)} \mathrm{Li}_q^{(a)}(u)\,\mathrm{Li}_r^{(b)}(u)\,\frac{\mathrm{d}u}{u}.\end{aligned} \tag{82}$$

We were able to use formula (82), together with formulas (17) through (20)—and related machinery described earlier in Section 3—to produce high-precision numerical values of the omega constants listed above in (69) through (75).

Alternatively, one may substitute $u = e^{-x}$ in formula (81) and obtain the following proposition.

Proposition 2 (Depth three computation)**.** *For $q \geq 0, r \geq 0, s > 0$, with $q + r + s > 2$, and $a \geq 0, b \geq 0, c \geq 0$ we have*

$$\begin{aligned}\omega_{a,b,c}(q,r,s) &= \int_0^1 \left(\frac{(-\log u)^{s-1}}{\Gamma(s)}\right)^{(c)} \mathrm{Li}_q^{(a)}(u)\,\mathrm{Li}_r^{(b)}(u)\,\frac{\mathrm{d}u}{u} \\ &= \int_0^{1/e} \left(\frac{(-\log u)^{s-1}}{\Gamma(s)}\right)^{(c)} \mathrm{Li}_q^{(a)}(u)\,\mathrm{Li}_r^{(b)}(u)\,\frac{\mathrm{d}u}{u} \\ &\quad + \int_{1/e}^1 \left(\frac{(-\log u)^{s-1}}{\Gamma(s)}\right)^{(c)} \mathrm{Li}_q^{(a)}(u)\,\mathrm{Li}_r^{(b)}(u)\,\frac{\mathrm{d}u}{u} \qquad (83) \\ &= \sum_{n,m>0} \left(\frac{\Gamma(s, n+m)}{\Gamma(s)\,(n+m)^s}\right)^{(c)} \frac{(-1)^n \log^a(n)}{n^q}\,\frac{(-1)^m \log^b(m)}{m^r} \\ &\quad + \int_{1/e}^1 \left(\frac{(-\log u)^{s-1}}{\Gamma(s)}\right)^{(c)} \mathrm{Li}_q^{(a)}(u)\,\mathrm{Li}_r^{(b)}(u)\,\frac{\mathrm{d}u}{u}, \qquad (84)\end{aligned}$$

where in (84) we express the result in terms of the incomplete Gamma function.

We have

$$\omega\left(\begin{array}{c|c} r & s \\ a & b \end{array}\right) = \zeta^{(a+b)}(r+s). \tag{85}$$

Now let $\zeta_{a,b}$ denote the partial derivative of the multi-zeta function

$$\zeta_{a,b}(r,s) := \sum_{k>j>0} \frac{(-\log k)^a}{k^r} \frac{(-\log j)^b}{j^s}.$$

Proposition 3 (Depth three reductions)**.** *For $s,t>0, a,b\geq 0$ by definition we have:*

$$\omega\left(\begin{array}{cc|c} 0, & 0 & t \\ 0, & 0 & b \end{array}\right) = \zeta^{(b)}(t) - \zeta^{(b)}(t-1) \tag{86}$$

$$\omega\left(\begin{array}{cc|c} s, & 0 & t \\ a, & 0 & b \end{array}\right) = \zeta_{b,a}(t,s) \tag{87}$$

$$\omega\left(\begin{array}{cc|c} s, & t & 0 \\ a, & b & 0 \end{array}\right) = \zeta^{(a)}(s)\,\zeta^{(b)}(t). \tag{88}$$

Moreover, from Euler's reflection formula [14]

$$\zeta(s,t)+\zeta(t,s) = \zeta(s)\zeta(t) - \zeta(t+s), \tag{89}$$

we obtain

$$\omega\left(\begin{array}{cc|c} s, & 0 & t \\ a, & 0 & b \end{array}\right) + \omega\left(\begin{array}{cc|c} t, & 0 & s \\ a, & 0 & b \end{array}\right) = \zeta^{(a)}(s)\,\zeta^{(b)}(t) - \zeta^{(a+b)}(t+s). \tag{90}$$

or equivalently

$$\omega\left(\begin{array}{cc|c} s, & t & 0 \\ a, & b & 0 \end{array}\right) - \omega\left(\begin{array}{cc|c} t, & 0 & s \\ a, & 0 & b \end{array}\right) - \omega\left(\begin{array}{cc|c} s, & 0 & t \\ a, & 0 & b \end{array}\right) = \zeta^{(a+b)}(t+s). \tag{91}$$

When $s=1$ (90) has singularities and must be handled with care. We fully address this issue in Theorem 8 and Corollary 2.

From (76) we see less trivial derivative relations lie within $\mathcal{D}$ than within $\mathcal{D}_1$. Four (of the seven) values given in Example 2 were degenerate: $\omega_{1,1,0}(1,0,3), \omega_{1,1,0}(2,0,2)$, and $\omega_{1,0,1}(1,0,3), \omega_{1,0,1}(2,0,2)$. In our earlier study, these were computed by other expedients described in [27]. In cases (72), (73) we may use a special case of (81), namely,

$$\omega_{a,0,b}(s,0,t) = \zeta_{b,a}(t,s) = \int_0^1 \left(\frac{(-\log x)^{t-1}}{\Gamma(t)}\right)^{(b)} \frac{\mathrm{Li}_s^{(a)}(x)}{1-x}\,\mathrm{d}x \tag{92}$$

with $a=b=2$, $s+t=4$ and $s=1,2$. Here $\zeta_{b,a}(t,s)$ again denotes partial derivatives of the multi-zeta function, and the notation $(\cdot)^{(b)}$ denotes the b-th partial derivative of the expression in parentheses with respect to t.

One may instead use

$$\Gamma(t)\zeta_{0,a}(t,s) = \int_0^1 (-\log x)^{t-1} \frac{\mathrm{Li}_s^{(a)}(x)}{1-x}\,\mathrm{d}x$$

and as before employ Leibnitz' formula to obtain

$$\zeta_{b,a}(t,s) = -\sum_{k=0}^{b-1} \binom{b}{k} \frac{\Gamma^{(b-k)}(b)}{\Gamma(b)} \zeta_{k,a}(t,s) + \int_0^1 \frac{\mathrm{Li}_s^{(a)}(x)}{1-x} \frac{\log^b(-\log x)}{\Gamma(b)} (-\log x)^{t-1}\,\mathrm{d}x \tag{93}$$

which leads to a nice ladder for computing $\zeta_{k,a}$ values using the algorithm already provided for $\Gamma^{(k)}$. The same process leads more generally, for $q+r+s>2$ and $a,b,b,q,r,s\ge 0$, to

$$\omega_{a,b,c}(q,r,s) = -\sum_{k=0}^{c-1}\binom{c}{k}\frac{\Gamma^{(c-k)}(c)}{\Gamma(c)}\omega_{a,b,k}(q,r,s) \\ + \frac{1}{\Gamma(c)}\int_0^1 \frac{\mathrm{Li}_q^{(a)}(x)\mathrm{Li}_r^{(b)}(x)}{x}\log^c(-\log x)(-\log x)^{s-1}\,\mathrm{d}x. \tag{94}$$

We emphasize that when computing quantities such as (69), (70), or say $\omega_{2,2,0}(1,1,2)$, we require the full version of (82) or (83).

4.5 Computation of the $\mathcal{U}$ constants in $\mathcal{D}_1$

In [8] for resolution of log-gamma integrals especially, we need MTW sums using only parameters 1 or 0. We define $\mathcal{U}(m,n,p,q)$ to vanish if $mn=0$; otherwise if $m\ge n$ we define

$$\mathcal{U}(m,n,p,q) := \frac{1}{2\pi}\int_0^{2\pi}\mathrm{Li}_1\left(e^{i\theta}\right)^{m-p}\mathrm{Li}_1^{(1)}\left(e^{i\theta}\right)^{p}\mathrm{Li}_1\left(e^{-i\theta}\right)^{n-q}\mathrm{Li}_1^{(1)}\left(e^{-i\theta}\right)^{q}\,\mathrm{d}\theta \\ = \omega\left(\begin{array}{c|c} \mathbf{1}_m & \mathbf{1}_n \\ \mathbf{1}_p\mathbf{0}_{m-p} & \mathbf{1}_q\mathbf{0}_{n-q}\end{array}\right), \tag{95}$$

while for $m<n$ we swap both (m,n) and (p,q) in the integral and the ω-generator. We then denoted the subensemble $\mathcal{D}_1\subset\mathcal{D}$ as the set $\mathcal{D}_1 := \{\mathcal{U}(m,n,p,q)\ :\ p\le m\ge n\ge q\}$. Another subensemble $\mathcal{D}_0\subset\mathcal{D}_1\subset\mathcal{D}$ comprises the *derivative-free* MTWs: $\mathcal{D}_0 := \{\mathcal{U}(M,N,0,0)\ :\ M\ge N\ge 1\}$; an element of $\mathcal{D}_0$ has the form $\omega(\mathbf{1}_M\mid\mathbf{1}_N)$, which can be thought of as an ensemble member as in (6) with all 1's across the top and all 0's across the bottom. Members of $\mathcal{D}_1$ were fully analyzed in [8].

5 Prior numerical investigations

Both to check our theory and evaluations, and to further explore the constants and functions being analyzed, we made many numerical computations in [8]. We recall a few of these prior experiments.

5.1 Relations amongst $\mathcal{U}$ constants

We computed, to 3100-digit precision, all of the $\mathcal{U}$ constants in $\mathcal{D}_1$ up to degree 10 (i.e., whose indices sum to 10 or less), according to the defining formula (95) and the rules given for $\mathcal{D}_1$ in Section 4.5. In particular, we calculated $\mathcal{U}(m,n,p,q)$ with $m,n\ge 1$, $m\ge n$, $m\ge p$, $n\ge q$, $m+n+p+q\le 10$. Our program found that there are 149 constants in this class. These computations, as above, were performed using the ARPREC arbitrary precision software [12] and the tanh-sinh quadrature algorithm (64), employing formulas (8), (9), (25) and (27) to evaluate the underlying polylog and polylog derivatives; and formulas (28), (30), (31) and (32) to evaluate the underlying zetas and derivatives.

We then searched among this set of numerical values for linear relations, using the multipair "PSLQ" integer relation algorithm [11], [16, pg. 230–234]. Our program first found the following relations, confirmed to over 3000-digit precision:

$$0 = \mathcal{U}(M,M,p,q) - \mathcal{U}(M,M,q,p), \tag{96}$$

for $M \in [1,4]$ and $2M+p+q \in [2,10]$, a total of 11 relations. That the programs uncover these simple symmetry relations gave us confidence that our software was working properly.

The programs then produced the following more sophisticated set of relations:

$$\begin{aligned}
0 &= 6\,\mathcal{U}(2,2,0,0) - 11\,\mathcal{U}(3,1,0,0) \\
0 &= 160\,\mathcal{U}(3,3,0,0) - 240\,\mathcal{U}(4,2,0,0) + 87\,\mathcal{U}(5,1,0,0) \\
0 &= 1680\,\mathcal{U}(4,4,0,0) - 2688\,\mathcal{U}(5,3,0,0) + 1344\,\mathcal{U}(6,2,0,0) - 389\,\mathcal{U}(7,1,0,0) \\
0 &= 32256\,\mathcal{U}(5,5,0,0) - 53760\,\mathcal{U}(6,4,0,0) + 30720\,\mathcal{U}(7,3,0,0) - 11520\,\mathcal{U}(8,2,0,0) \\
&\quad + 2557\,\mathcal{U}(9,1,0,0).
\end{aligned} \tag{97}$$

Upon completion, our PSLQ program reported an *exclusion bound* of 2.351×10^{19}. This means that in any integer linear relation among the set of 149 constants that is not listed above, the Euclidean norm of the corresponding vector of coefficients must exceed 2.351×10^{19}. Under the hypothesis that linear relations only are found among constants of the same degree, we obtained exclusion bounds of at least 3.198×10^{73} for each degree in the tested range (degree 4 through 10).

5.2 Computational notes I

The entire computation, including quadrature and PSLQ calculations, required 94,727 seconds run time on one core of a 2012-era Apple *MacPro* workstation. Of this run time, initialization (including the computation of zeta and zeta derivative values, and precalculating values of $\mathrm{Li}_1(e^{i\theta})$ and $\mathrm{Li}_1'(e^{i\theta})$ at abscissa points specified by the tanh-sinh quadrature algorithm [13]) required 82074 seconds. After initialization, the 149 quadrature calculations completed quickly (a total of 6894 seconds), as did the 16 PSLQ calculations (a total of 5760 seconds). These relations were established by using *Maple*. For instance, $\mathcal{U}(3,1,0,0) = 6\,\zeta(4)$, and $\mathcal{U}(2,2,0,0) = 11\,\zeta(4)$, which establishes the first relation in (**??**). The third relation in (**??**) follows similarly.

5.2.1 A conjecture proven

From the equations in (**??**) we *conjectured* that (i) there is one such relation at each even weight $(4,6,8,\ldots)$ and none at odd weight, and (ii) in each case $p=q=0$. Thus, there appear to be no nontrivial relations between derivatives outside $\mathcal{D}_0$ but in $\mathcal{D}_1$. Any negative results must perforce be empirical as one cannot at the present prove things even as "simple" as the irrationality of $\zeta(5)$.

Accordingly, we performed a second computation :using 780-digit arithmetic and only computing elements of a given weight d, where $4 \le d \le 20$, with $m+n=d$ and $p=q=0$. The PSLQ search then quickly returned the additional relations culminating with:

$$\begin{aligned}
0 =& -147995367744824832\mathcal{U}(10,10,0,0) + 269082486269542400\mathcal{U}(11,9,0,0) \\
&- 201811864702156800\mathcal{U}(12,8,0,0) + 124191916739788800\mathcal{U}(13,7,0,0) \\
&- 62095958369894400\mathcal{U}(14,6,0,0) + 24838383347957760\mathcal{U}(15,5,0,0) \\
&- 7761994796236800\mathcal{U}(16,4,0,0) + 1826351716761600\mathcal{U}(17,3,0,0) \\
&- 304391952793600\mathcal{U}(18,2,0,0) + 32041258191552\mathcal{U}(19,1,0,0)
\end{aligned} \tag{98}$$

No relations were found when the degree was odd, aside from trivial relations such as $\mathcal{U}(7,8,0,0) = \mathcal{U}(8,7,0,0)$. For all weights, except for the above-conjectured relations, no others were found, with exclusion bounds of at least 2.481×10^{75}.

Remark 7. The above conjecture (at least the even-weight part) has been proven in [8]. Even the generating-function algebra was motivated by numerics—i.e. we had to seek some kind of unifying structure for the $\mathcal{U}$ functions. This in turn made more general results accessible. $\Diamond$

6 Current numerical investigations

Given our success in computationally analyzing the $\mathcal{U}$ constants in [8], and prompted by the example evaluation (76), we decided to extend our computer programs to evaluate and analyze more general ω constants, namely those with higher-order polylogarithm derivatives. To that end we have employed the machinery developed in Section 3 along with formulas (82) and (83).

Our *null hypothesis* is that all relations are explained by Theorem 5, Proposition 3, and simple symmetries. That is, in light of our earlier paper and preliminary explorations, we anticipated finding only relations consistent with the theorems and methods of Section 4. We eschewed using (86) as it leads to—probably unhelpful—inhomogeneous relations.

6.1 Computational experiments

In light of Proposition 3 and of (76) we first computed $\omega_{a,b,c}(q,r,s)$ constants for derivative weight $D = a + b + c$, where $1 \le D \le 4$ and argument weight $W = q + r + s$, where $3 \le W \le 5$ (these are depth three constants; we deferred higher-level constants to another study). We then searched for relations among these constants. In a single large PSLQ run, involving all these constants, we found many relations, but in each case, the derivative weight D and the argument weight W of each term in the relation was constant. We found no relations where the derivative weight D of each term didn't match, nor where the argument weight W of terms varied.

Thus, we focused our more detailed analyses of these relations on cases with fixed W and D. To that end, we performed the following steps:

Algorithm 1 (Relation detection)**.** Our program performed the following steps:

1. For a given derivative weight $D = a + b + c$, and a given argument weight $W = q + r + s$, we first computed, to 200-digit precision, all $\omega_{a,b,c}(q,r,s)$ for this D and W, except in cases that are clearly related to already-computed constants.

   Example: For $D = 4$, $W = 5$, we did not compute $\omega_{1,1,2}(2,0,3)$, since $\omega_{1,1,2}(0,2,3)$ was already in the table, and the two are equal by symmetry; also, we did not compute $\omega_{1,2,1}(1,1,3)$, since it equals $\omega_{1,2,1}(0,1,4) + \omega_{1,2,1}(1,0,4)$ by (67).

2. After outputting 200-digit numerical values for all constants, we deleted those from the list those which, as noted in the previous item, are related to already-computed constants in the list by elementary relations.

3. We then ran the two-level multipair PSLQ program [11] on the resulting list of terms.

4. For each PSLQ-discovered relation, we first tried to further reduce the relation by applying simple formulas such as (67). Then after outputting the relation, we deleted the last-indexed term of the discovered relation and re-ran PSLQ.

5. When no more relations were found, we then augmented the list of remaining terms with one constant of the form $\zeta^{(D)}(W)$, or $\zeta^{(d_1)}(w_1)\zeta^{(d_2)}(w_2)$ with $d_1 + d_2 = D$ and $w_1 + w_2 = W$. If a relation was found using the PSLQ routine, then this term was deleted from the list, and another zeta constant of this form was added, until the list of zeta terms was exhausted and no relations could be found by the PSLQ routine among the remaining constants.

We present in Table 1 sample PSLQ-discovered relations for the case $W = 4$ and $D = 5$. Note that relations (99) through (101) involve only omega constants, whereas relations (102) through (108) each involves one zeta constant.

Remark 8. We note that even these remaining relations can, as far as we know, with some effort be manually proved using the rigorously proven results given in this paper. Automating this process has proven harder than we anticipated—but equality verification in a computer algebra system is known to be very hard; see [10].

For example, relations (104) and (108) are nothing more than instances of Proposition 3. Thence, based on these results, the "null hypothesis" mentioned above has not been disproven. $\lozenge$

We summarize in Table 2 some overall statistics of these runs, including the total number of omega terms and zeta terms, the number of relations found (simple and PSLQ-discovered), and the final number of linearly independent terms (i.e., the size of the underlying residual basis). There are clearly suggestive patterns in this data, for which more study is needed..

6.2 Computational notes II

This exercise underscored the need for additional research and development of highly efficient software to compute a wide range of special functions to arbitrarily high precision, across the full range of complex arguments (not just for a limited range of real arguments). We relied largely on our own computer programs and the ARPREC arbitrary precision software in this study in part because, as noted, we were unable to obtain the needed functionality in commercial software.

For instance, neither *Maple* nor *Mathematica* was able to numerically evaluate the $\mathcal{U}_1$ and ω constants to high precision in reasonable run time, in part because of the challenge of computing polylog and polylog derivatives at real and complex arguments, and in part because of the cost of performing high-precision quadrature. For example, the version of *Mathematica* that we were using was able to numerically evaluate $\partial \mathrm{Li}_s(z)/\partial s$ to high precision, but such evaluations were hundreds of times slower than the evaluation of $\mathrm{Li}_s(z)$ itself, and, in some cases, did not return the expected number of correct digits. In some cases, *Mathematica* returned the requested precision, but only a handful digits were correct. Additionally, as noted, the versions of *Mathematica* we used inexplicably refused to produce numerical values of $\zeta^{(n)}(0)$ for $n \geq 4$.

Finally, we found that our ARPREC-based computer codes (implemented at the high level in Fortran-90, then automatically translated to the C++ library of low-level ARPREC routines) were hundreds of times faster than similar codes implemented in *Mathematica*. We do not fully understand the full reason for this difference, but given that our ARPREC-based codes were sufficiently fast to perform this research satisfactorily, we had little reason to pursue the question.

Remark 9. One binding feature on these computations is the number of terms needed in Theorems 1 and 2 to obtain a given level of precision in the numerical values of the polylogarithm functions. In our computations, we found this number to be somewhat greater than the number of decimal

$$
\begin{aligned}
0 &= \omega_{0,1,3}(0,2,3) - \omega_{0,1,3}(0,3,2) - \omega_{0,3,1}(0,2,3) + \omega_{0,3,1}(0,3,2) \\
&\quad - \omega_{1,3,0}(0,2,3) - \omega_{1,3,0}(0,3,2) + \omega_{1,3,0}(2,0,3) + \omega_{1,3,0}(3,0,2) && (99)\\
0 &= -\omega_{0,1,3}(0,2,3) + \omega_{0,2,2}(0,2,3) + \omega_{0,2,2}(0,3,2) - \omega_{0,3,1}(0,3,2) \\
&\quad - 6\omega_{2,2,0}(0,1,4) - 3\omega_{2,2,0}(0,2,3) - \omega_{2,2,0}(0,3,2) + \omega_{1,3,0}(2,3,0) && (100)\\
0 &= -3\omega_{0,0,4}(0,1,4) + \omega_{0,0,4}(0,2,3) + 2\omega_{0,0,4}(0,3,2) + \omega_{0,4,0}(0,2,3) \\
&\quad + 3\omega_{0,4,0}(0,3,2) - \omega_{0,4,0}(1,1,3) - 3\omega_{0,4,0}(2,1,2) - 2\omega_{0,4,0}(3,1,1) && (101)
\end{aligned}
$$

$$
\begin{aligned}
0 &= -\omega_{0,0,4}(0,1,4) - \omega_{0,0,4}(0,2,3) + 3\omega_{0,1,3}(0,2,3) + 3\omega_{0,3,1}(0,3,2) \\
&\quad - \omega_{0,1,3}(0,3,2) - \omega_{0,3,1}(0,2,3) + \omega_{1,3,0}(3,0,2) + \omega_{0,4,0}(1,2,2) \\
&\quad + \omega_{0,4,0}(2,3,0) - \omega_{1,3,0}(2,1,2) - \omega_{1,3,0}(2,2,1) - 3\omega_{1,3,0}(2,3,0) + 2\zeta^{(4)}(5) && (102)\\
0 &= -\omega_{0,0,4}(0,2,3) + \omega_{0,0,4}(0,3,2) - \omega_{0,4,0}(2,1,2) - \omega_{0,4,0}(3,1,1) \\
&\quad + 2\omega_{0,4,0}(1,2,2) - 2\zeta^{(4)}(5) && (103)\\
0 &= \zeta^{(0)}(2)\zeta^{(4)}(3) - \omega_{0,4,0}(2,3,0) && (104)\\
0 &= -\omega_{0,1,3}(0,2,3) - \omega_{0,3,1}(0,3,2) + 4\zeta^{(1)}(2)\zeta^{(3)}(3) \\
&\quad - \omega_{0,1,3}(0,3,2) - \omega_{0,3,1}(0,2,3) + \omega_{1,3,0}(3,0,2) - \omega_{1,3,0}(2,1,2) \\
&\quad - \omega_{1,3,0}(2,2,1) - 3\omega_{1,3,0}(2,3,0) && (105)\\
0 &= \omega_{0,0,4}(0,2,3) - 2\omega_{0,2,2}(0,2,3) - 2\omega_{0,2,2}(0,3,2) + 2\zeta^{(2)}(2)\zeta^{(2)}(3) \\
&\quad + \omega_{0,0,4}(0,3,2) - \omega_{0,4,0}(1,1,3) - \omega_{0,4,0}(2,2,1) - \omega_{0,4,0}(3,2,0) && (106)\\
0 &= \omega_{0,0,4}(0,2,3) - 2\omega_{0,1,3}(0,3,2) - 2\omega_{0,3,1}(0,2,3) + 2\zeta^{(3)}(2)\zeta^{(1)}(3) \\
&\quad + \omega_{0,0,4}(0,3,2) - \omega_{0,4,0}(1,1,3) - \omega_{0,4,0}(2,2,1) - \omega_{0,4,0}(3,2,0) && (107)\\
0 &= \zeta^{(4)}(2)\zeta^{(0)}(3) - \omega_{0,4,0}(3,2,0) && (108)
\end{aligned}
$$

Table 1: Relations found for $\omega_{a,b,c}(q,r,s)$ with $W = a+b+c = 4$ and $D = q+r+s = 5$.

D	W	Omega terms	Zeta terms	Relations	Residual basis
1	3	30	3	24	9
1	4	30	4	23	11
1	5	45	5	37	13
2	3	36	4	22	18
2	4	60	5	48	22
2	5	90	7	70	27
3	3	60	5	36	29
3	4	100	7	70	37
3	5	150	9	114	45
4	4	150	8	102	56
4	5	225	11	167	69

Table 2: Statistics for relation searches

digits required in the results. This number then governed, in turn, the number of values of $\zeta^{(m)}(k+1-n)$, $c_{k,j}(\mathcal{L})$, $b_{k,j}(\mathcal{L})$, $f_{k,q}$ that must be precomputed. The precision level itself was determined by the large number of terms in the PSLQ searches mentioned above. As noted above, for PSLQ to reliably recover a relation $(a_1, a_2, \cdots, a_n)$ of length n, where the coefficients (a_i) have maximum absolute value 10^d, requires at least dn-digit precision in the input vector, and at least dn-digit arithmetic in the operation of the algorithm. Along this line, once PSLQ finds a relation, one should delete an element of the resulting relation before continuing, in additional PSLQ runs, to find other relations. In this way, the number of terms for PSLQ can be reduced to more manageable levels for finding the hard-to-recover relations, resulting in significantly faster total run times. $\Diamond$

6.3 Some rigorous consequences

Analysis of the experimental results suggested the following theorem.

Theorem 8. *For all $a > 0$ we have*

$$\begin{aligned}
\zeta\left(a+2\right) &= \omega(a,1,1) - \zeta(a+1,1) \qquad (109)\\
&= \frac{1}{\Gamma\left(a+1\right)} \int_0^1 \frac{\left(-\log\left(u\right)\right)^a \left(-\log\left(1-u\right)\right)}{\left(1-u\right)} \, \mathrm{d}u \\
&\quad - \int_0^1 \mathrm{Li}_a\left(u\right) \frac{\left(-\log\left(1-u\right)\right)}{u} \, \mathrm{d}u \qquad (110)
\end{aligned}$$

Proof. We sketch the proof and will provide a fuller proof as part of a later paper. We use a classical result due to Fritz D. Carlson (from his 1914 dissertation [24]) on discrete analytic continuation. The first published proof was given in [35, §5.81]. An accessible proof of a special case broad enough for our application, due to Selberg, is presented in [1, p. 112].

By Carlson's theorem it suffices to show that (109) holds for positive integers. But in this case we may expand $\omega(a,1,1)$ using Theorem 5—or directly summing $\zeta(m,n) = \omega(m,1,n-1) - \omega(m-1,1,n)$—to reduce (109) to

$$\zeta(a+2) = \sum_{m=2}^{a+1} \zeta(m, a+2-m),$$

which, for perforce integer a, is a well known result for MZVs [14].

Equation (110) then follows from the integral representations given above. $\square$

Remark 10. Theorem 8 was discovered by observing multiple small-value cases of (113). On computing the exponential generating function of both sides of (113), we were led directly to (109). Likewise, for $a \geq 0$

$$\omega\left(a,2,1\right) = \zeta\left(a+1,2\right) + \zeta\left(2,a+1\right) - \zeta\left(a+2,1\right) \qquad (111)$$

may be derived from (109) or proven as it was. $\Diamond$

From Theorem 8 we deduce many of the experimentally observed relations involving zeta derivatives at integer values.

Corollary 1 (Derivative evaluations)**.** *For $n = 0, 1, 2, \ldots$ and every $a > 0$ we have*

$$\zeta^{(n)}(a+2) = \omega^{(n)}(a,1,1) - \zeta^{(n)}(a+1,1), \tag{112}$$

or, in full ω notation,

$$\zeta^{(n)}(a+2) = \omega_{n,0,0}(a,1,1) - \omega_{0,0,n}(1,0,a+1). \tag{113}$$

In like fashion from (111) we obtain

$$\omega^{(n)}(a,2,1) = \zeta_{n,0}(a+1,2) + \zeta_{0,n}(2,a+1) - \zeta_{n,0}(a+2,1) \tag{114}$$

for $a > 0$ and $n = 1, 2, \ldots$.

Also, on comparing Corollary 2 to Euler's reflection formula (89) we deduce that:

Corollary 2 (Removable singularity)**.** *For $n = 0, 1, 2, \ldots$ and every $a > 0$ we have*

$$\begin{aligned} \zeta^{(n)}(a+2) + \zeta^{(n)}(a+1,1) &= \omega^{(n)}(a,1,1) \\ &= \lim_{b \downarrow 1} \zeta(b)\,\zeta^{(n)}(a+1) - \zeta^{(n)}(b,a+1). \end{aligned} \tag{115}$$

Remark 11. For integer $m > 0$, equation (109) can be rewritten as

$$\omega(m,1,1) = \frac{m+3}{2}\,\zeta(m+2) - \frac{1}{2}\sum_{k=2}^{m} \zeta(k)\zeta(m+2-k), \tag{116}$$

on applying Euler's reduction of $\zeta(a,1)$, as given in [14]. $\diamondsuit$

Thus, our null hypothesis has been upheld, albeit refined as in Corollaries 1 and 2.

6.4 Future computations

In light of these experiments, we think it unlikely that there are any qualitatively different relations for $r + s + t \geq 6$. We also presume, with less confidence, that the situation remain similar for higher depth sums $\omega_{a_1,\ldots,a_n}(s_1,\ldots,s_n)$. In light of the computational effort needed for experiments with higher derivatives, we intend instead to (i) try to further automate our process; and then to (ii) look at at the non-degenerate weight four case with $N = 2$; and to (iii) explore depth four $\omega_{a,b,c,d}(q,r,s,t)$.

7 Conclusion

This study underscores the need for high-precision evaluations of special functions in much research. This need spurred the late Richard Crandall to compile a set of unified and rapidly convergent algorithms (some new, some gleaned from existing literature) for a variety of special functions, fitted for practical implementation and efficient for very high-precision computation [27]. Crandall's work has been in part described and extended by the current authors in [7].

Since, as we have illustrated, the polylogarithms and their relatives are central to a great deal of mathematics and mathematical physics [4, 21, 31], such an effort is bound to pay off in the near future. Indeed it is the basis for a 2014–2016 Australian Research Council Discovery Project by the current authors in tandem with Richard Brent. We conclude by emphasising that our research agenda is driven as much by the desire to improve tools for computer-assisted discovery as it is by the precise needs of the current project.

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