Computation and theory of extended Mordell-Tornheim-Witten sums

David H. Bailey* Jonathan M. Borwein† Richard E. Crandall‡

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Abstract

We consider some fundamental generalized Mordell–Tornheim–Witten (MTW) zeta-function values along with their derivatives, and explore connections with multiple-zeta values (MZVs). To achieve these results, we make use of symbolic integration, high precision numerical integration, and some interesting combinatorics and special-function theory. Our original motivation was to represent previously unresolved constructs such as Eulerian log-gamma integrals. Indeed, we are able to show that all such integrals belong to a vector space over an MTW basis, and we also present, for a substantial subset of this class, explicit closed-form expressions. In the process, we significantly extend methods for high-precision numerical computation of polylogarithms and their derivatives with respect to order.

- The associated paper is at http://carmasite.newcastle.edu.au/jon/MTW1.pdf.

*Lawrence Berkeley National Laboratory, Berkeley, CA 94720, DHBailey@lbl.gov.

†Centre for Computer-assisted Research Mathematics and its Applications (CARMA), School of Mathematical and Physical Sciences, University of Newcastle, Callaghan, NSW 2308, Australia. Email: jonathan.borwein@newcastle.edu.au, jborwein@gmail.com.

‡Center for Advanced Computation, Reed College. Email: crandall@reed.edu

1 PART I: Introduction

We define an ensemble of extended Mordell–Tornheim–Witten (MTW) zeta function values [19, 35, 23, 24, 5, 12, 36, 37]. 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 include *derivatives with respect to the order* of the terms. We also investigate interrelations between MTW evaluations, and explore some deeper connections with multiple-zeta values (MZVs). To achieve these results, we make use of 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. Indeed, we consider an algebra having an MTW basis together with the constants $\pi, 1/\pi, \gamma, \log 2\pi$ and the rationals, and show that every log-gamma integral

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

is an element of said algebra (that is, a finite superposition of MTW values with fundamental-constant coefficients). That said, the focus of our paper is the relation between MTW sums and classical polylogarithms. It is the adumbration of these relationships that makes the study significant.

The organization of the talk is as follows.

PART I. In Section 2 we introduce an ensemble $\mathcal{D}$ capturing the values we wish to study and we provide some effective integral representations in terms of polylogarithms on the unit circle. In Section 2.1 we introduce a subensemble $\mathcal{D}_1$ sufficient for the study log gamma integrals, while in Section 2.2 we provide a first few accessible closed forms. In Section 3 we provide generating functions for various derivative free MTW sums and provide proofs of results first suggested by numerical experiments described in the sequel. In Section 4 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 have to first provide similar tools for the zeta function and its derivatives at integer points. These methods are of substantial independent value and will be pursued in a future paper.

PART II. In Section 5 we prove various reductions and interrelations of our MTW values (see Theorems 7, 8, 9 and 10). In Theorem 11 of Section 6, we show how to evaluate all log gamma integrals $\mathcal{LG}_n$ for $n = 1, 2, 3 \ldots$, in terms of our special ensemble of MTW values, and we confirm our expressions to at least 400-digit precision. In Section 7 we describe two rigorous experiments designed to use *integer relation methods* [13] to first explore the structure of the ensemble $\mathcal{D}_1$ and then to begin to study $\mathcal{D}$. Finally, in Section 8 we make some summary remarks.

My only picture: an Australian blob fish

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 [29], but remains mysterious with respect to many combinatorial phenomena, especially when we contemplate derivatives with respect to the s_i parameters. We 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 an apparently novel generalized MTW zeta function for positive integers M, N and nonnegative integers s_i, t_j—with constraints $M \ge N \ge 1$—together with a polylogarithm-integral representation:

$$\omega(s_1,\ldots,s_M \mid t_1,\ldots,t_N) := \sum_{\substack{m_1,\ldots,m_M,n_1,\ldots,n_N>0\\ \sum_{i=1}^M m_i=\sum_{j=1}^N n_j}} \prod_{i=1}^M \frac{1}{{m_i}^{s_i}} \prod_{j=1}^N \frac{1}{{n_j}^{t_j}} \tag{2}$$

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

Here the *polylogarithm of order* s denotes $\mathrm{Li}_s(z) := \sum_{n\ge1} z^n/n^s$ and its analytic extensions [28] and the (complex) number s is its *order*.

It is important to note that if some parameter(s) is (are) zero, there are convergence issues with this integral representation. One may either use principal-value calculus, or use an alternative representation such as (11) below. When $N = 1$ the representation (3) devolves to the classic MTW form, in the sense that

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

In the present study we shall require a wider *MTW ensemble* involving outer derivatives, according to the notation

$$\begin{aligned}\omega\begin{pmatrix} s_1, \ldots, s_M & \mid & t_1, \ldots, t_N \\ d_1, \ldots, d_M & \mid & e_1, \ldots e_N \end{pmatrix} &:= \sum_{\substack{m_1,\ldots,m_M,n_1,\ldots,n_N>0 \\ \sum_{i=1}^M m_i = \sum_{j=1}^N n_j}} \prod_{i=1}^M \frac{(-\log m_i)^{d_i}}{{m_i}^{s_i}} \prod_{j=1}^N \frac{(-\log n_j)^{e_j}}{{n_j}^{t_j}} \\ &= \frac{1}{2\pi} \int_0^{2\pi} \prod_{i=1}^M \mathrm{Li}_{s_i}^{(d_i)}\left(e^{i\theta}\right) \prod_{j=1}^N \mathrm{Li}_{t_j}^{(e_j)}\left(e^{-i\theta}\right) \, \mathrm{d}\theta,\end{aligned} \tag{5}$$

where the s-th outer derivative of a polylogarithm is denoted $\mathrm{Li}_s^{(d)}(z) := \left(\frac{\partial}{\partial s}\right)^d \mathrm{Li}_s(z)$.

The aforementioned work [5] represents such numbers differently but equivalently—by placing the d, e parameters as a string subscript on ω. (We opt presently for the $(M+N) \times 2$ matrix parameterization because some recondite expressions will accrue for which the matrix structure is somewhat more readable.) 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 thus far, we consider an MTW ensemble, meaning the set of numbers

$$\mathcal{D} := \left\{ \omega\begin{pmatrix} s_1, \ldots, s_M & \mid & t_1, \ldots, t_N \\ d_1, \ldots, d_M & \mid & e_1, \ldots e_N \end{pmatrix} : \ s_i, d_i, t_j, e_j \geq 0; \ M \geq N \geq 1, M, N \in \mathbb{Z}^+ \right\}. \tag{6}$$

2.1 Important subensembles

We shall have occasion, in our resolution of log-gamma integrals especially, to contemplate MTW constructs possessed only of parameters 1 or 0. We define $\mathcal{U}(m,n,p,q)$ to vanish if $mn=0$; otherwise if $m \geq n$ we define

$$\begin{aligned} \mathcal{U}(m,n,p,q) &:= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{Li}_1\left(e^{i\theta}\right)^{m-p} \mathrm{Li}_1^{(1)}\left(e^{i\theta}\right)^{p} \mathrm{Li}_1\left(e^{-i\theta}\right)^{n-q} \mathrm{Li}_1^{(1)}\left(e^{-i\theta}\right)^{q} \,\mathrm{d}\theta \\ &= \omega\begin{pmatrix} \mathbf{1}_m & \mid & \mathbf{1}_n \\ \mathbf{1}_p\mathbf{0}_{m-p} & \mid & \mathbf{1}_q\mathbf{0}_{n-q} \end{pmatrix}, \end{aligned} \tag{7}$$

while for $m<n$ we swap both (m,n) and (p,q) in the integral and the ω-generator. We then denote a particular subensemble $\mathcal{D}_1 \subset \mathcal{D}$ as the set

$$\mathcal{D}_1 \;:=\; \{\mathcal{U}(m,n,p,q) \;:\; p \leq m \geq n \geq q\}.$$

Furthermore, another subensemble $\mathcal{D}_0 \subset \mathcal{D}_1 \subset \mathcal{D}$ is a *derivative-free* set of MTWs of the form

$$\mathcal{D}_0 \;:=\; \{\mathcal{U}(M,N,0,0) \;:\; M \geq N \geq 1\},$$

that is to say, 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 (5) with all 1's across the top and all 0's across the bottom. As this work progressed it became clear that we should also treat

$$\mathcal{D}_0(s) \;:=\; \{\mathcal{U}_s(M,N,0,0) \;:\; M \geq N \geq 1\},$$

in which an element of $\mathcal{D}_0(s)$ has the form $\omega(\mathbf{s}_M \mid \mathbf{s}_N)$, for $s=1,2,\ldots$. Of course $\mathcal{D}_0(1)=\mathcal{D}_0$. For economy of notation, we shall write

$$\mathcal{U}_s(M,N) := \mathcal{U}_s(M,N,0,0).$$

2.2 Closed forms for certain MTWs

We consider first some relatively elementary evaluations. For $N = 1$ in the definition (5) we have the following:

$$\omega(r \mid s) = \zeta(r+s), \tag{8}$$

$$\omega(r_1, \ldots, r_M \mid 0) = \prod_{j=1}^{M} \zeta(r_j) \tag{9}$$

$$\omega(r, 0 \mid s) = \omega(0, r \mid s) = \zeta(s, r), \tag{10}$$

where this last entity is a multiple-zeta value (MZV), some instances of which—such as $\zeta(6,2)$ have never been resolved in closed form [14] and are believed *irreducible*, see also [10, 36, 37]. Such beginning evaluations use simple combinatorics; later in Section 5 we shall see much more sophisticated combinatorics come into play.

When we are derivative-free and $N = 1$, so that we are contemplating the original, classic MTW (1), there is a useful pure-real integral available as an alternative to integral representation (3). In fact,

$$\omega(s_1, s_2, \ldots, s_M \mid t) = \frac{1}{\Gamma(t)} \int_0^\infty x^{t-1} \prod_{j=1}^{M} \mathrm{Li}_{s_j}(e^{-x})\, \mathrm{d}x. \tag{11}$$

It is intriguing that this real representation can be split into a series plus a numerically easier incomplete Gamma function integral, as discussed in [22]. Specifically, with a free parameter λ, one has

$$\omega(s_1, s_2, \ldots, s_M \mid t) = \frac{1}{\Gamma(t)} \int_0^\lambda x^{t-1} \prod_{j=1}^{M} \mathrm{Li}_{s_j}(e^{-x})\, \mathrm{d}x + \frac{1}{\Gamma(t)} \sum_{m_1,\ldots,m_M \geq 1} \frac{\Gamma(t, \lambda(m_1 + \cdots + m_M))}{m_1^{s_1} \cdots m_M^{s_M}\ (m_1 + m_2 + \cdots m_M)^t}, \tag{12}$$

which recovers the full integral as $\lambda \to \infty$ (11).

But numerics aside, there are interesting symbolic machinations that employ (11). For example, since

$$\mathrm{Li}_0(z) = \frac{z}{1-z},$$

we have a 1-parameter MTW value

$$\omega(0,0,0,0 \mid t) = \frac{1}{\Gamma(t)} \int_0^\infty \frac{x^{t-1}}{(e^x - 1)^4}\, \mathrm{d}x = -\zeta(t) + \frac{11}{6}\zeta(t-1) - \zeta(t-2) + \frac{1}{6}\zeta(t-3),$$

certainly valid for $t > 4$. It is amusing and instructive that multidimensional analytic continuation is patently nontrivial. Indeed, the analytic continuation for $t \to 0$ here appears to be $\omega(0,0,0,0 \mid 0) \stackrel{?}{=} \frac{251}{720}$, and yet from the zeta-product formula previous we might infer instead $\omega(0,0,0,0 \mid 0) = \zeta(0)^4 \stackrel{?}{=} \frac{1}{16}$.

This shows that analytic continuation of MTWs (as indeed with MZVs) must be performed carefully and rigorously [26, 29, 33].

At any rate, it can be shown, via these definite-integration techniques or sheer combinatorics, that when the argument t is in its region of absolute convergence, we have the attractive closed form

$$\omega(\mathbf{0}_M \mid t) = \frac{1}{(M-1)!} \sum_{q=1}^{M} s(M,q)\, \zeta(t-q+1), \tag{13}$$

where the $s(M, q)$ are the *Stirling numbers of the first kind* [32] as discussed prior to (77).

3 Resolution of all $\mathcal{U}(M, N)$ and more

Whereas our previous section exhibits closed forms for $N = 1$ (i.e. some classic MTW forms of the type (4)), there is an important class of resolvable MTWs where N is allowed to roam freely.

3.1 An exponential generating function for $\mathcal{U}(M, N)$

Consider the subensemble $\mathcal{D}_0$ from Section 2.1; that is, the MTW is derivative-free with all 1's across the top row. The following results, which were experimentally motivated as we see later—provide a remarkably elegant generating function for $\mathcal{U}(m, n) := \mathcal{U}(m, n, 0, 0)$.

Theorem 1 (Generating function for $\mathcal{U}$). *We have a formal generating function for $\mathcal{U}$ as defined by (7) with $p, q = 0$; namely,*

$$\mathcal{V}(x, y) := \sum_{m,n\geq 0} \mathcal{U}(m, n)\, \frac{x^m\, y^n}{m!\, n!} \;=\; \frac{\Gamma(1-x-y)}{\Gamma(1-x)\Gamma(1-y)}. \tag{14}$$

Proof. To see this starting with the integral form in (7), we exchange integral and summation and then make an obvious change of variables to arrive at

$$\mathcal{V}(x,y) = \frac{2^{-x-y+1}}{\pi}\int_0^{\pi/2} (\cos\theta)^{-x-y}\cos\left((x-y)\,\theta\right)\,\mathrm{d}\theta. \tag{15}$$

However, for Re $a > 0$ [32, Equation (5.12.5)] records the beta function evaluation:

$$\int_0^{\pi/2} (\cos\theta)^{a-1}\cos(b\theta)\,\mathrm{d}\theta = \frac{\pi}{2^a}\frac{1}{a\,\mathrm{B}\left(\frac{1}{2}(a+b+1),\frac{1}{2}(a-b+1)\right)}. \tag{16}$$

On setting $a = 1-x-y, b = x-y$ in (16) we obtain (14). □

Note that setting $y = \pm x$ in (14) leads to two natural one dimensional generating functions. For instance

$$\mathcal{V}(x,-x) = \sum_{m,n\geq 1} (-1)^n \binom{m+n}{n} \mathcal{U}(m,n)\,\frac{x^{m+n}}{(m+n)!} \;=\; \frac{\sin(\pi x)}{\pi x}. \tag{17}$$

Example 1. Theorem 1 makes it very easy to evaluate $\mathcal{U}(m,n)$ symbolically as the following *Maple* squib illustrates.

```
UU := proc (m, n) local x, y, H;
   H := proc (x,y) ->GAMMA(x+y+1)/(GAMMA(x+1)*GAMMA(y+1));
   subs(y=0,diff(subs(x=0,diff(H(-x,-y),`$`(x, n))),`$`(y, m)));
 value(%) end proc
```

For instance, UU(5,5) returns:

$$9600\,\pi^2\zeta\,(5)\,\zeta\,(3) + 600\,\zeta^2\,(3)\,\pi^4 + \frac{77587}{8316}\,\pi^{10} + 144000\,\zeta\,(7)\,\zeta\,(3) + 72000\,\zeta^2\,(5)\,. \tag{18}$$

This can be done in *Maple* on a current *Lenovo* in a fraction of a second, while the 61 terms of $\mathcal{U}(12,12)$ were obtained in 1.31 seconds and the 159 term expression for $\mathcal{U}(15,15)$ took 14.71 seconds and to 100 digits has numerical value of

$$\begin{aligned} &8.81079181877873690464902067277676666735325622358992908192916 20963 \\ &95561049543747340201380539725128849 \times 10^{31}. \end{aligned} \tag{19}$$

This was fully in agreement with our numerical integration scheme of the next section. $\Diamond$

The *log-sine-cosine integrals* given by

$$\operatorname{Lsc}_{m,n}(\sigma) := \int_0^\sigma \log^{m-1}\left|2\,\sin\frac{\theta}{2}\right|\,\log^{n-1}\left|2\,\cos\frac{\theta}{2}\right|\,d\theta \tag{20}$$

have been considered by Lewin, [27, 28] and in physical applications, see for instance [25]. From the form given in [11], Lewin's result can be restated as

$$\mathcal{L}(x,y) := \sum_{m,n=0}^{\infty} 2^{m+n}\operatorname{Lsc}_{m+1,n+1}(\pi)\,\frac{x^m}{m!}\frac{y^n}{n!} = \pi\binom{2x}{x}\binom{2y}{y}\frac{\Gamma(1+x)\,\Gamma(1+y)}{\Gamma(1+x+y)}. \tag{21}$$

This is closely linked to (14), see also [34]. Indeed, we may rewrite (21) as

$$\mathcal{L}(x,y)\,\mathcal{V}(-x,-y) = \pi\binom{2x}{x}\binom{2y}{y}. \tag{22}$$

3.2 An exponential-series representation of the generating function $\mathcal{V}$

To proceed with analyses on the generating function $\mathcal{V}(x, y)$, we recall expansions of the Gamma function itself. To this end, we note from [27, 32] the classical formula

$$\begin{aligned} \log \Gamma(1-z) &= \gamma z + \sum_{n>1} \zeta(n) \frac{z^n}{n}, \\ e^{-\gamma z} \Gamma(1-z) &= \exp\left\{ \sum_{n>1} \frac{\zeta(n) z^n}{n} \right\}, \end{aligned} \tag{23}$$

everything being convergent for $|z| < 1$.

This leads immediately to a powerful exponential-series representation for our generating function

$$\begin{aligned} \mathcal{V}(x, y) &= \frac{\Gamma(1-x-y)}{\Gamma(1-x)\Gamma(1-y)} = \exp\left\{ \sum_{n>1} \frac{\zeta(n)}{n} \left((x+y)^n - x^n - y^n \right) \right\} \\ &= \exp\left\{ \sum_{n>1} \frac{\zeta(n)}{n} \sum_{k=1}^{n-1} \binom{n}{k} x^k y^{n-k} \right\}. \end{aligned} \tag{24}$$

These combinatorics lead directly to a resolution of the $\mathcal{D}_0$ ensemble, in the sense of casting every $\mathcal{U}(M, N)$ is a finite, closed form:

Theorem 2 (Evaluation of $\mathcal{U}(M,N)$). *For any integers $M \geq N \geq 1$ we have that*

$$\mathcal{U}(M,N) \ = \omega(\mathbf{1}_M \mid \mathbf{1}_N) \ \in \mathcal{D}_0$$

lies in the ring generated as

$$\mathcal{R} \ := \ \langle \mathcal{Q} \cup \{\pi\} \cup \{\zeta(3), \zeta(5), \zeta(7), \ldots\} \rangle \, .$$

In particular, for $M \geq N$, and setting $\mathcal{U}(M,0) := 1$, the general expression is:

$$\mathcal{U}(M,N) \ = \ M!\,N! \sum_{n=1}^{N} \frac{1}{n!} \sum_{\substack{j_1+\cdots+j_n=M \\ k_1+\cdots+k_n=N}} \prod_{i=1}^{n} \frac{(j_i+k_i-1)!}{j_i!\,k_i!} \, \zeta(j_i+k_i).$$

Hence, any such $\mathcal{U}$ element is expressible in terms of odd zeta values, rationals, and the constant π, with every zeta product involved having weight $M+N$.[1]

Proof. All results follow from symbolic Taylor expansion of the exponential form (24); that is, denote by Q the quantity in the braces $\{\ \}$ of the exponent in (24). Then inspection of $\exp\{Q\} = 1 + Q + Q^2/2! + \ldots$ gives a finite form for a coefficient $\mathcal{U}(M,N)$. □

Actually, there is a second proof that again connects the present theory with log-sine integrals:

[1]We refer to a ring, not a vector space over ζ values, as it can happen that *powers* of a ζ can appear; thus we need closure under multiplication of any generators.

Proof. (Alternative proof of Theorem 2) From the logarithmic form of Li_1 (61), we have

$$\mathcal{U}(M,N) = \frac{(-1)^{M+N}}{2\pi} \times \int_0^{2\pi} \left(\log\left(2\sin\frac{t}{2}\right) - \frac{(\pi-t)}{2}i\right)^M \left(\log\left(2\sin\frac{t}{2}\right) + \frac{(\pi-t)}{2}i\right)^N \mathrm{d}t. \tag{25}$$

Now, upon expanding the integrand we can cast this $\mathcal{U}$ as a finite superposition of log-sine integrals. Specifically, from [16] we employ

$$\mathrm{Ls}_{n+k+1}^{(k)}(2\pi) \;:=\; -\int_0^{2\pi} t^k \log^n\left(2\sin\left(\frac{t}{2}\right)\right) \mathrm{d}t.$$

Indeed, Borwein and Straub [16] provide a full generating function:

$$\mathrm{Ls}_{n+k+1}^{(k)}(2\pi) \;=\; -2\pi(-i)^k \left(\frac{\partial}{\partial u}\right)^k \left(\frac{\partial}{\partial \lambda}\right)^{n+k+1} e^{i\pi u}\binom{\lambda}{\lambda/2+u} \Big|_{\{u,\lambda\}=\{0,0\}},$$

from which provably closed form computation becomes possible. The rest of the proof can follow along the lines of the first proof; namely, one only need inspect the exponential-series expansion for the combinatorial bracket. ☐

Example 2 (Sample $\mathcal{U}$ values)**.** Exemplary evaluations are

$$\begin{aligned}
\mathcal{U}(4,2) &= \omega(1,1,1,1\,|1,1) \;=\; 204\,\zeta(6) + 24\,\zeta(3)^2,\\
\mathcal{U}(4,3) &= \omega(1,1,1,1\,|1,1,1) \;=\; 6\,\pi^4\zeta(3) + 48\,\pi^2\zeta(5) + 720\,\zeta(7),\\
\mathcal{U}(6,1) &= \omega(1,1,1,1,1,1\,|1) \;=\; 720\,\zeta(7),
\end{aligned}$$

the latter consistent with a general evaluation that can be achieved in various ways,

$$\mathcal{U}(M,1) \;=\; \omega(\mathbf{1}_M \mid 1) \;= M!\,\zeta(M+1), \tag{26}$$

valid for all $M = 1, 2, \ldots$. Note that all terms in each decomposition have the same weight $M+N$ (seven in the final two cases). ◊

3.3 Sum rule for the $\mathcal{U}$ functions

Remarkably, extreme-precision numerical experiments as detailed in a later section discovered a unique sum rule amongst $\mathcal{U}$ functions with a fixed *even* order $M+N$. Eventually, we were led to by such numerical discoveries to prove:

Theorem 3. *(Sum rule for $\mathcal{U}$ of even weight) For even $p > 2$ we have*

$$\sum_{m=2}^{p-2} (-1)^m \binom{p}{m} \mathcal{U}(m, p-m) \;=\; 2p\left(1 - \frac{1}{2^p(p+1)B_p}\right)\mathcal{U}(p-1,1), \tag{27}$$

where B_p is the p-th Bernoulli number.

Proof. Equating powers of x on each side of the contraction $\mathcal{V}(x,-x)$ (relation (17)), and using the known evaluation $\mathcal{U}(p-1,1) = (p-1)!\,\zeta(p)$ together with the Bernoulli form of $\zeta(p)$ (given as relation (65)), the sum rule is obtained. □

Example 3 (Theorem 3 for weight $M+N=20$)**.** For $M+N=20$, the theorem gives *precisely the numerically discovered relation* (133). As we shall see, empirically it is the unique such relation at that weight. An idea as to the rapid growth of the sum-rule coefficients is this: For weight $M+N=100$, the integer relation coefficient of $\mathcal{U}(50,50)$ is even, and exceeds 7×10^{140}; note also (26). ◊

3.4 Further conditions for ring membership

For more general real $c>b$, the integral representation

$$\omega(\mathbf{1}_a\,\mathbf{0}_b \mid c) \;=\; \frac{(-1)^{a+c-1}}{\Gamma(c)}\int_0^1 \frac{(1-u)^{b-1}}{u^b}\log^{c-1}(1-u)\log^a u\,\mathrm{d}u, \tag{28}$$

is finite and we remind ourselves that the a ones and b zeros can be permuted in any way. While such integrals are covered by Theorem 10 below, its special form allows us to show there is a reduction of (28) entirely to sums of one-dimensional zeta products—despite the comment in [28, §7.4.2]—since we may use the partial derivatives of the beta function, denoted $B_{a,c-1}$, to arrive at:

Theorem 4. *For non-negative integers a,b,c with $c>b$, the number $\omega(\mathbf{1}_a\,\mathbf{0}_b \mid c)$ lies in the ring $\mathcal{R}$ from Theorem 2, and so reduces to combinations of ζ values.*

Proof. One could proceed using exponential-series methods as for Theorem 2 previous, but this time we choose to use Gamma-derivative methods, in a spirit of revealing equivalence between such approaches. From (28) we have, formally,

$$(-1)^{a+c-1}\Gamma(c)\,\omega(\mathbf{1}_a\,\mathbf{0}_b\mid c) = \lim_{u\to -b}\frac{\partial}{\partial v^{(c-1)}}\left\{\frac{\partial}{\partial u^a}\frac{\Gamma(u+1)\Gamma(v)}{\Gamma(u+v+1)}\right\}_{v=b} \tag{29}$$

The analysis simplifies somewhat on expanding $(1-u)^{b-1}/u^b$ by the binomial theorem. so that the ω value in question is a finite superposition of terms

$$I(a,b,c) := \int_0^1 \frac{\log^c(1-u)\log^a u}{u^b}\,\mathrm{d}u = \lim_{u\to -b}\frac{\partial}{\partial v^c}\left\{\frac{\partial}{\partial u^a}\frac{\Gamma(u+1)\Gamma(v)}{\Gamma(u+v+1)}\right\}_{v=1}. \tag{30}$$

Thence, we obtain the asserted complete reduction to sums of products of one-dimensional zeta functions via the exponential-series arguments of the previous section or by appealing to known properties of poly-gamma functions [16], [27, §7.9.5] and [31, §5.15]. More details can be found in [10, pp. 281–282] and [27, §7.9.2]. $\square$

Remark 1. We note that [27, (7.128)] give $I(2,1,2) = 8\,\zeta\,(5) - \frac{2}{3}\,\zeta\,(3)\,\pi^2$ and an incorrect value for $I(3,1,2) = 6\,\zeta^2\,(3) - \frac{1}{105}\,\pi^6$. $\diamondsuit$

Example 4. Representative evaluations are

$$\omega(1,1,1,0,0\mid 3) = (\pi^2-12)\,\zeta(3) - 3\,\zeta(3)^2 - 18\,\zeta(5) + \pi^2 + \frac{\pi^4}{12} + \frac{\pi^6}{210}, \tag{31}$$

and

$$\omega(1,1,0,0,0\mid 5) = \left(\frac{7}{4} - \frac{11\pi^2}{12} - \frac{\pi^4}{36}\right)\zeta(3) + \frac{9\zeta(3)^2}{2} + \frac{29\zeta(5)}{2} - \frac{2\pi^2\zeta(5)}{3} + 10\zeta(7) - \frac{\pi^4}{16} - \frac{\pi^6}{144}. \tag{32}$$

Now, not all terms have the same weight. $\diamondsuit$

3.5 The subensemble $\mathcal{D}_0(s)$

Given the successful discovery of $\mathcal{V}$ in Section 3.2, we turn to $\mathcal{D}_0(s)$ from Section 2.1. We define $\mathcal{U}_s(0,0)=1$, $\mathcal{U}_s(m,n)$ for $s=1,2,3,\ldots$ to vanish if $m>n=0$; otherwise if $m\geq n$ we set

$$\mathcal{U}_s(m,n) := \frac{1}{2\pi}\int_0^{2\pi} \mathrm{Li}_s\left(e^{i\theta}\right)^m \mathrm{Li}_s\left(e^{-i\theta}\right)^n \,\mathrm{d}\theta \;=\; \omega\left(\begin{array}{c|c} \mathbf{s}_m & \mathbf{s}_n \\ \mathbf{0}_m & \mathbf{0}_n \end{array}\right). \tag{33}$$

That is, we consider derivative free elements of $\mathcal{D}$ of the form $\omega(\mathbf{s}_M \mid \mathbf{s}_N)$. An obvious identity is

$$\mathcal{U}_s(1,1)=\zeta(2s). \tag{34}$$

Likewise

$$\mathcal{U}_s(2,1)=\omega(s,s,s), \tag{35}$$

which is evaluable by Theorem 7 and for which classical closed forms are recorded in [23, Eqns (1.20) and (1.21)]. Likewise, $\mathcal{U}_s(n,1)$ is evaluable for positive integer n.

For $p=2$, we obtain a corresponding exponential generating function

$$\mathcal{V}_2(x,y) := \sum_{m,n\geq 0} \mathcal{U}_2(m,n)\,\frac{x^m\,y^n}{m!\,n!}. \tag{36}$$

Whence, summing and exchanging integral and sum as with $p=1$, we get

$$\begin{aligned}\mathcal{V}_2(ix,iy) :=\ & \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{(y-x))\mathrm{Cl}_2(\theta)}\, \cos\left(\frac{(2\,\pi^2+3\,\theta^2-6\,\pi\,\theta)}{12}\,(y+x)\right)\, \mathrm{d}\theta \\ &+ i\,\frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{(y-x))\mathrm{Cl}_2(\theta)}\, \sin\left(\frac{(2\,\pi^2+3\,\theta^2-6\,\pi\,\theta)}{12}\,(y+x)\right)\, \mathrm{d}\theta \end{aligned} \tag{37}$$

where $\mathrm{Cl}_2(\theta) := -\int_0^{\theta} \log\left(2\left|\sin\frac{t}{2}\right|\right)\, \mathrm{d}t$ is the Clausen function [28, Ch. 4]. While it seems daunting to place this in fully closed form, we can evaluate $\mathcal{V}_2(x,x)$. It transpires, in terms of the *Fresnel integrals* S and C [32, §7.2(iii)], to be

$$\begin{aligned}2\pi\,\mathcal{V}_2(ix,ix) =\ & 2\sqrt{\frac{\pi}{x}}\left(\cos\left(\frac{x\pi^2}{6}\right) C\left(\sqrt{\pi x}\right) + \sin\left(\frac{x\pi^2}{6}\right) S\left(\sqrt{\pi x}\right)\right) \\ &+ i\,2\sqrt{\frac{\pi}{x}}\left(\cos\left(\frac{x\pi^2}{6}\right) S\left(\sqrt{\pi x}\right) - \sin\left(\frac{x\pi^2}{6}\right) C\left(\sqrt{\pi x}\right)\right). \end{aligned} \tag{38}$$

On using the series representations [32, Eq. (7.6.4) & (7.6.6)] we arrive at:

$$\begin{aligned}\mathrm{Re}\ \mathcal{V}_2(ix,ix) =\ & \cos\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^{\infty} \frac{(-1)^n\,\pi^{4\,n}}{2^{2\,n+2}\,(2\,n)!\,(4\,n+1)}\,x^{2\,n} \\ &+ \sin\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^{\infty} \frac{(-1)^n\,\pi^{4\,n+2}}{2^{2\,n+3}\,(2\,n+1)!\,(4\,n+3)}\,x^{2\,n+1}, \end{aligned} \tag{39}$$

and

$$\begin{aligned}\mathrm{Im}\ \mathcal{V}_2(ix,ix) =\ & -\sin\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^{\infty} \frac{(-1)^n\,\pi^{4\,n}}{2^{2\,n+2}\,(2\,n)!\,(4\,n+1)}\,x^{2\,n} \\ &+ \cos\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^{\infty} \frac{(-1)^n\,\pi^{4\,n+2}}{2^{2\,n+3}\,(2\,n+1)!\,(4\,n+3)}\,x^{2\,n+1}. \end{aligned} \tag{40}$$

We note that $\mathrm{Re}\mathcal{V}_2(ix,ix)$ is an even function and $\mathrm{Im}\mathcal{V}_2(ix,ix)$ is odd. On comparing (36) with $ix = iy$ to (39) or (40) we arrive that:

Theorem 5. *(Sum rule for $\mathcal{U}_2$) For each integer $p \geq 1$, there are explicit positive rational numbers q_p such that*

$$\sum_{m=1}^{2p-1} \binom{2p}{m} \mathcal{U}_2(m, 2p-m) = (-1)^p\, q_{2p}\, \pi^{4p}, \tag{41}$$

$$\sum_{m=1}^{2p} \binom{2p+1}{m} \mathcal{U}_2(m, 2p+1-m) = (-1)^p\, q_{2p+1}\, \pi^{4p+2}. \tag{42}$$

Example 5 (Relations with $s = 2$)**.** We note that unlike the case of $s = 1$ we have obtained a relation of each weight! This will happen whenever s is even. The rational numbers q_n are easy to compute symbolically from (38). Thence, to order 16:

$$\begin{aligned}\mathcal{V}_2(ix,ix) = 1 &- \frac{1}{90}\pi^4 x^2 + \frac{1}{22680}\pi^8 x^4 - \frac{53}{525404880}\pi^{12} x^6 + \frac{19}{128619114624}\pi^{16} x^8 \\ &+ \left(-\frac{1}{2835}\pi^6 x^3 + \frac{1}{561330}\pi^{10} x^5 - \frac{1}{262702440}\pi^{14} x^7\right) + \cdots .\end{aligned} \tag{43}$$

These illustrate how much unexpected structure one might hope to uncover within $\mathcal{D}$. We will give exact formulas for the coefficients of (43) in (49) and (50) below. ◊

Remark 2. There is additional useful information to be gleaned from (37). Setting $y = -x$, we deduce that

$$\mathcal{V}_2(ix, -ix) = \frac{1}{\pi}\int_0^{\pi} \cos\left(\mathrm{Cl}_2(\theta)\, 2x\right)\, \mathrm{d}\theta. \tag{44}$$

Comparing coefficients on each side, we obtain linear combinations of $\mathcal{U}_2$ sums adding up to $C_{2n} := \frac{1}{\pi}\int_0^{\pi} \mathrm{Cl}_2(\theta)^{2n}\, \mathrm{d}\theta$ for each positive integer n. While $C_1 = \mathrm{Ls}_3^{(1)}(\pi)$ [17], no closed form seems to be known for any such C_{2n}. ◊

3.5.1 The $\mathcal{U}_s$ sums when $s \geq 3$

It is possible to undertake the same analysis generally. For instance, from the evaluation Gl_3 [28, Eqn (22), p. 297] may deduce that

$$\mathcal{V}_3(x,-x) = \frac{1}{\pi}\int_0^\pi \cos\left(\left(\pi^2-\theta^2\right)\frac{\theta}{6}\,x\right)\,\mathrm{d}\theta. \tag{45}$$

The Taylor series commences

$$\mathcal{V}_3(x,-x) = 1 - \frac{1}{945}\,\pi^6x^2 + \frac{1}{3648645}\,\pi^{12}x^4 - \frac{1}{31819833045}\,\pi^{18}x^6 + O\left(x^8\right).$$

Again the order-two coefficient is in agreement with (34). Note also that $6\,\mathcal{U}_3(2,1)$ is the next coefficient and that all terms have the weight one would predict.

In general, we exploit the *Glaisher functions*, $\mathrm{Gl}_{2n}(\theta) := \mathrm{Re}\,\mathrm{Li}_{2n}\left(e^{i\theta}\right)$ and $\mathrm{Gl}_{2n+1}(\theta) := \mathrm{Im}\,\mathrm{Li}_{2n+1}\left(e^{i\theta}\right)$. They possess closed forms:

$$\mathrm{Gl}_n\left(\theta\right) = (-1)^{1+\lfloor n/2\rfloor}2^{n-1}\frac{\pi^n}{n!}\,B_n\left(\frac{\theta}{2\pi}\right) \tag{46}$$

for $n>1$ where B_n is the n-th *Bernoulli polynomial* [28, Eqn. (22), p 300] and $0\leq\theta\leq 2\pi$. Thus,

$$\mathrm{Gl}_5\left(\theta\right) = \frac{1}{720}\,t\left(\pi-t\right)\left(2\,\pi-t\right)\left(4\,\pi^2+6\,\pi\,t-3\,t^2\right).$$

We then observe that:

$$\mathcal{V}_{2n+1}(x,-x) = \frac{1}{2\pi}\int_0^{2\pi} \cos\left(\mathrm{Gl}_{2n+1}\left(e^{i\theta}\right)x\right)\,\mathrm{d}\theta, \tag{47}$$

$$\mathcal{V}_{2n}(ix,ix) = \frac{1}{2\pi}\int_0^{2\pi} \exp\left(i\left(\mathrm{Gl}_{2n}\left(e^{i\theta}\right)x\right)\right)\,\mathrm{d}\theta. \tag{48}$$

In each case substitution of (46) and term-by-term expansion of cos or sin leads to an expression for the coefficients—note that $\mathrm{Gl}_n(\theta)$ is an homogeneous two-variable polynomial in π and θ with each monomial of degree n. Indeed, we are thus led to explicit formulas

$$r_m(s) := (-1)^m \frac{4^{m-1}}{(2m)!\,\pi}\int_0^{2\pi}\left(\frac{(-1)^{1+\lfloor s/2\rfloor}}{s!}(2\pi)^s B_n\left(\frac{\theta}{2\pi}\right)\right)^{2m}\mathrm{d}\theta \tag{49}$$

$$i_m(s) := (-1)^m \frac{2\,4^{m-1}}{(2m+1)!\,\pi}\int_0^{2\pi}\left(\frac{(-1)^{1+\lfloor s/2\rfloor}}{s!}(2\pi)^s B_n\left(\frac{\theta}{2\pi}\right)\right)^{2m+1}\mathrm{d}\theta. \tag{50}$$

for the real and imaginary coefficients of order $2m$. (While we may expand these as finite sums, they may painlessly be integrated symbolically.) The imaginary coefficient is zero for s odd.

Thence, we have established:

Theorem 6 (Sum relations for $\mathcal{U}_s$)**.** *Let s be a positive integer. There is an analogue of Theorem 3 when s is odd and of Theorem 5 when s is even.*

Example 6 (Relations with $s=2$ revisited)**.** In *Maple* we have the code:

```
cor:=(s,m)->int(4^m*Gln(s,theta)^(2*m)/(2*m)!,theta=0..2*Pi)/2/Pi;


coi:=(s,m)->int(4^m*2*Gln(s,theta)^(2*m+1)/(2*m+1)!,theta=0..2*Pi)/2/Pi;
```

For $s=2$ we recover

```
> add((-1)^k*cor(2,k)*x^(2*k),k=0..4);
             1   2   4     1     8  4      53        12  6
        1 - -- x  Pi  + ----- Pi  x  - --------- Pi   x
            90          22680          525404880


                  19        16  8
           + ------------ Pi   x
             128619114624
> add((-1)^k*coi(2,k)*x^(2*k),k=0..3);
          1     6  2     1      10  4       1       14  6
       - ---- Pi  x  + ------ Pi   x  - --------- Pi   x
         2835          561330           262702440
```

for the real and imaginary coefficients of x^{2n}, exactly as in (39) and (40). $\diamond$

As in of Remark 2, we may also adduce that integrals of powers of n-th order Clausen functions appear as linear combinations of U_n sums.

4 Fundamental computational expedients

To numerically study the ensemble $\mathcal{D}$ intensively, we must be able to differentiate polylogarithms with respect to their order. Even for our primary goal herein —- the study of $\mathcal{D}_1$ — we need access to the first derivative of Li_1.

4.1 Polylogarithms and their derivatives with respect to order

In regard to the needed polylogarithm values, reference [5] gives formulas such as the following: when $s = n$ is a positive integer,

$$\mathrm{Li}_n(z) = \sum_{m=0}^{\infty}{}' \zeta(n-m)\frac{\log^m z}{m!} + \frac{\log^{n-1} z}{(n-1)!}\left(H_{n-1} - \log(-\log z)\right), \tag{51}$$

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,

$$\mathrm{Li}_s(z) = \sum_{m\geq 0} \zeta(s-m)\frac{\log^m z}{m!} + \Gamma(1-s)(-\log z)^{s-1}. \tag{52}$$

Note in formula (51), the condition $|\log z| < 2\pi$ precludes the usage of this formula for computation when $|z| < e^{-2\pi} \approx 0.0018674$. For such small $|z|$, however, it suffices to use the definition

$$\mathrm{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s}. \tag{53}$$

In fact, we found that formula (53) is generally faster than (51) whenever $|z| < 1/4$, at last for precision levels in the range of 100 to 4000 digits.

4.1.1 Derivatives of general order polylogarithms

For positive integer k we have a formula in [22, §9, eqn. (51)]: for $|\log z| < 2\pi$ and $\tau \in [0, 1)$:

$$\mathrm{Li}_{k+1+\tau}(z) = \sum_{0 \le n \ne k} \zeta(k+1+\tau-n)\frac{\log^n z}{n!} + \frac{\log^k}{k!}\sum_{j=0}^{\infty} c_{k,j}(\mathcal{L})\,\tau^j, \tag{54}$$

where $\mathcal{L} := \log(-\log z)$ and the c coefficients engage the Stieltjes constants [22, §7.1]:

$$c_{k,j}(\mathcal{L}) = \frac{(-1)^j}{j!}\gamma_j - b_{k,j+1}(\mathcal{L}). \tag{55}$$

Here the $b_{k,j}$ terms are given by

$$b_{k,j}(\mathcal{L}) := \sum_{\substack{p+t+q=j\\ p,t,q\ge 0}} \frac{\mathcal{L}^{\,p}}{p!}\frac{\Gamma^{(t)}(1)}{t!}(-1)^{t+q} f_k(q), \tag{56}$$

where $f_k(q)$ is the coefficient of x^q in $\prod_{m=1}^{k} \frac{1}{1+x/m}$, easily calculable via $f_{k,0} = 1$ and the recursion

$$f_{k,q} = \sum_{h=0}^{q} \frac{(-1)^h}{k^h} f_{k-1,q-h}. \tag{57}$$

Then, $f_{k,1} = -H_k$ and $f_{k,2} = \frac{1}{2}H_k^2 + \frac{1}{2}H_k^{(2)}$ — in terms of generalized harmonic numbers — while $c_{k,0} = H_k - \mathcal{L}$. With $k = \tau = 0$ this yields (51).

To obtain first (or higher) derivatives $\mathrm{Li}_{k+1}^{(1)}(z)$, we differentiate (54) at zero and so require the evaluation $c_{k,1}$. With $k = 0$ and $j = 1$ this supplies (59) below.

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

Most importantly, we may write, for $0 < \theta \leq 2\pi$,

$$\mathrm{Li}_1(e^{i\theta}) = -\log\left(2\sin\left(\frac{\theta}{2}\right)\right) + \frac{(\pi-\theta)}{2}i. \tag{58}$$

As described above, the order derivatives $\mathrm{Li}'_s(z) = \mathrm{d}(\mathrm{Li}_s(z))/\,\mathrm{d}s$ for integer s, can be computed with formulas such as

$$L'_1(z) = \sum_{n=1}^{\infty} \zeta'(1-n)\frac{\log^n z}{n!} - \gamma_1 - \frac{1}{12}\pi^2 - \frac{1}{2}\left(\gamma + \log(-\log z)\right)^2, \tag{59}$$

which, as before, is valid whenever $|\log z| < 2\pi$. Here γ_1 is the *second Stieltjes constant* [3, 22]. For small $|z|$, it again suffices to use the elementary form

$$\mathrm{Li}'_s(z) = -\sum_{n=1}^{\infty} \frac{z^k \log k}{k^s}. \tag{60}$$

Relation (59) can be applied to yield the formula

$$\mathrm{Li}'_1(e^{i\theta}) = \sum_{n=1}^{\infty} \zeta'(1-n)\frac{(i\theta)^n}{n!} - \gamma_1 - \frac{1}{12}\pi^2 - \frac{1}{2}\left(\gamma + \log(-i\theta)\right)^2, \tag{61}$$

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

With such formulas as above, to evaluate $\mathcal{U}$ values one has the option of contemplating either pure quadrature to resolve an element, a convergent series for same, or a combination of quadrature and series. All of these are gainfully exploited in the MTW examples of [22].

4.2 ζ at integer arguments

Using formulas (51) and (52) for computation requires precomputed values of the zeta function and its derivatives at integer arguments, see [3, 20]. One fairly efficient algorithm for computing $\zeta(n)$ for integer $n > 1$ is the following given by Peter Borwein [18]: Choose $N > 1.2 \cdot D$, where D is the number of correct digits required. Then

$$\zeta(s) \approx -2^{-N}(1-2^{1-s})^{-1} \sum_{i=0}^{2N-1} \frac{(-1)^i \sum_{j=-1}^{i-1} u_j}{(i+1)^s}, \tag{62}$$

where $u_{-1} = -2^N$, $u_j = 0$ for $0 \le j < N-1$, $u_{N-1} = 1$, and $u_j = u_{j-1} \cdot (2N-j)/(j+1-N)$ for $j \ge N$.

4.2.1 ζ at positive integer arguments

In our setting, given that we require $\zeta(n)$ for many integers $n > 1$, the following approach—adopted in [6]—is more efficient. First, to compute $\zeta(2n)$, observe that

$$\begin{aligned} \coth(\pi x) &= \frac{-2}{\pi x} \sum_{k=0}^{\infty} \zeta(2k)(-1)^k x^{2k} \\ &= \cosh(\pi x)/\sinh(\pi x) \\ &= \frac{1}{\pi x} \cdot \frac{1 + (\pi x)^2/2! + (\pi x)^4/4! + (\pi x)^6/6! + \cdots}{1 + (\pi x)^2/3! + (\pi x)^4/5! + (\pi x)^6/7! + \cdots}. \end{aligned} \tag{63}$$

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

$$R_{k+1}(x) := R_k(x) + [1 - Q(x) \cdot R_k(x)] \cdot R_k(x), \tag{64}$$

where both the degree of the polynomial and the numeric precision of the coefficients are dynamically increased, approximately doubling whenever convergence has been achieved at a given degree and precision, until the final desired degree and precision are achieved. When this process is complete, the quotient P/Q is simply the product $P(x) \cdot R(x)$. The required values $\zeta(2k)$ can then be obtained from the coefficients of this product polynomial as in [6]. Note that $\zeta(0) = -1/2$.

4.2.2 ζ at nonpositive integer arguments

The *Bernoulli numbers* B_{2k}, which are also needed, can then be obtained from the positive even-indexed zeta values by the formula [32, Eqn. (25.6.2)]

$$B_{2k} = (-1)^{k+1} \frac{2(2k)!\zeta(2k)}{(2\pi)^{2k}}. \tag{65}$$

The positive odd-indexed zeta values can be efficiently computed using these two Ramanujan-style formulas [6, 15]:

$$\begin{aligned} \zeta(4N+3) &= -2\sum_{k=1}^{\infty} \frac{1}{k^{4N+3}(\exp(2k\pi)-1)} \\ &\quad -\pi(2\pi)^{4N+2} \sum_{k=0}^{2N+2} (-1)^k \frac{B_{2k}B_{4N+4-2k}}{(2k)!(4N+4-2k)!}, \\ \zeta(4N+1) &= -\frac{1}{N}\sum_{k=1}^{\infty} \frac{(2\pi k + 2N)\exp(2\pi k) - 2N}{k^{4N+1}(\exp(2k\pi)-1)^2} \\ &\quad -\frac{1}{2N}\pi(2\pi)^{4N} \sum_{k=1}^{2N+1} (-1)^k \frac{B_{2k}B_{4N+2-2k}}{(2k-1)!(4N+2-2k)!}. \end{aligned} \tag{66}$$

Finally, the zeta function can be evaluated at negative integers by the following well-known formulas [32, (25.6.3),(25.6.4)]:

$$\zeta(-2n+1) = -\frac{B_{2n}}{2n} \qquad \text{and} \qquad \zeta(-2n) = 0. \tag{67}$$

4.3 ζ' at integer arguments

Precomputed values of the zeta derivative function are prerequisite for the efficient use of formulas (59) and (61).

4.3.1 ζ' at positive integer arguments

For positive integer arguments, the derivative zeta is well computed via a series-accelerated algorithm for the derivative of the eta or alternating zeta function, see (80). The scheme is illustrated in the following *Mathematica* code (for argument `ss` and precision `prec` digits). It is an adaptation of a scheme presented in [22] and based on more general acceleration methods in [21]:

```
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))]
```

Note that in this algorithm, the logarithm and zeta values can be precalculated, and so do not significantly add to the run time. Similar techniques apply to derivatives of η.

4.3.2 ζ' at nonpositive integer arguments

From the functional equation $\zeta(s) = 2(2\pi)^{s-1} \sin\frac{\pi s}{2}\,\Gamma(1-s)\,\zeta(1-s)$ one can extract

$$\zeta'(0) = -\frac{1}{2}\log 2\pi$$

and for even $m = 2, 4, 6, \ldots$

$$\zeta'(-m) := \frac{d}{ds}\zeta(s)|_{s=-m} = \frac{(-1)^{m/2} m!}{2^{m+1}\pi^m}\,\zeta(m+1) \tag{68}$$

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

$$\zeta'(-m) = \zeta(-m)\left(\gamma + \log 2\pi - H_m - \frac{\zeta'(m+1)}{\zeta(m+1)}\right). \tag{69}$$

Example 7 (Zeta first derivative values)**.** We obtain results such as

$$\zeta'(-4) = \frac{3}{4}\frac{\zeta(5)}{\pi^4},$$

and

$$\zeta'(-5) = \frac{15}{4\pi^6}\,\zeta'(6) + \frac{137}{15120} - \frac{\gamma}{252} - \frac{1}{252}\log 2\pi,$$

and so on. ◊

We shall examine different methods more suited to higher derivatives in the sequel.

4.4 Higher derivatives of ζ

To approach these we first need to attack the Gamma function.

4.4.1 Derivatives of Γ at positive integers

Let $g_n := \Gamma^{(n)}(1)$. Now it is well known [32, (5.7.1) and (5.7.2)] that

$$\Gamma(z+1)\,\mathcal{C}(z) = z\,\Gamma(z)\,\mathcal{C}(z) = z \tag{70}$$

where

$$\mathcal{C}(z) := \sum_{k=1}^{\infty} c_k z^k$$

with $c_0 = 0, c_1 = 1, c_2 = \gamma$ and

$$(k-1)c_k = \gamma c_{k-1} - \zeta(2)\,c_{k-2} + \zeta(3)\,c_{k-3} - \cdots + (-1)^k\,\zeta(k-1)\,c_1, \tag{71}$$

Thus, differentiating (70) by Leibniz' formula, for $n \geq 1$ we have

$$g_n = -\sum_{k=0}^{n-1} \frac{n!}{k!}\,g_k\,c_{n+1-k}. \tag{72}$$

More generally, for positive integer m we have

$$\Gamma(z+m)\ \mathcal{C}(z) = (z)_m \tag{73}$$

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 (73) and obtain

$$g_n(m) = -\sum_{k=0}^{n-1} \frac{n!}{k!}\, g_k(m)\, c_{n+1-k} + \frac{D_m^{n+1}}{n+1}. \tag{74}$$

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

$$D_m^n = \sum_{k=0}^{m-n} s\,(m, k+n)\,(k+1)_n\,(m-1)^k = (n+1)!\,(-1)^{m+n+1} s\,(m, 1+n)\,. \tag{75}$$

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

$$\frac{g_n(m)}{n!} = -\sum_{k=0}^{n-1} \frac{g_k(m)}{k!}\, c_{n+1-k} + |s(m,1+n)|. \tag{76}$$

where for integer $n, k \ge 0$

$$s(n,k) = s(n-1,k-1) - (n-1)\, s(n-1,k)\,, \tag{77}$$

see [32, Equation (26.8.18)].

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

For $n = 0, 1, 2, \ldots$, and with

$$\kappa := -\log(2\pi) - \tfrac{1}{2}\pi i,$$

we have Apostol's explicit formulas [32, (25.6.13) and (25.6.14)]:

$$(-1)^k \zeta^{(k)}(1-2n) = \frac{2(-1)^n}{(2\pi)^{2n}} \sum_{m=0}^{k} \sum_{r=0}^{m} \binom{k}{m} \binom{m}{r} \mathrm{Re}(\kappa^{k-m})\, \Gamma^{(r)}(2n)\, \zeta^{(m-r)}(2n)\,, \tag{78}$$

$$(-1)^k \zeta^{(k)}(-2n) = \frac{2(-1)^n}{(2\pi)^{2n+1}} \sum_{m=0}^{k} \sum_{r=0}^{m} \binom{k}{m} \binom{m}{r} \mathrm{Im}(\kappa^{k-m})\, \Gamma^{(r)}(2n+1)\, \zeta^{(m-r)}(2n+1) \tag{79}$$

.

Since in (74) only the initial conditions rely on m, equations (78) and (79) are well fitted to work with (74) (along with (77), and (71)).

4.4.3 η and its derivatives at negative integers

The alternating zeta function, whose computation at positive integer values was discussed obliquely in Section 4.3.1, is given by

$$\eta(s) := \left(1 - 2^{1-s}\right)\zeta(s) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n}. \tag{80}$$

We may then compute $\eta^{(n)}(m)$ for negative integer m from the product rule again

$$\eta^{(n)}(m) = \eta(m)\,\zeta^{(n)}(m) + 2^{1-m}\sum_{k=1}^{n}(-1)^k\binom{n}{k}\zeta^{(n-k)}(m)\log^k 2. \tag{81}$$

Conversely, as Lagrange duality will show,

$$\zeta^{(n)}(m) = \sum_{k=0}^{n}\binom{n}{k}\eta^{(n-k)}(m)\,D_k(m). \tag{82}$$

Here

$$D_k(s) \;:=\; \frac{\mathrm{d}^k}{\mathrm{d}s^k}\left(\frac{1}{1-2^{1-s}}\right) \;=\; \frac{-\log^k(2)}{\left(-1+2^{1-s}\right)^{k+1}}\sum_{j=0}^{k} E\left(k, j+1\right) 2^{(1-s)\cdot(k-j)}, \tag{83}$$

where $E(k,j)$ is the Eulerian number given recursively by $E(1,j) = \delta_1(j)$, $E(k,1) = 1$ and, for $k, j \geq 2$,

$$E(k,j) \;=\; jE(k-1,j) + (k-j+1)E(k-1,j-1), \tag{84}$$

or by

$$E(k,j) \;=\; \sum_{i=0}^{j}(-1)^i\binom{k+1}{i}(j-i)^k\,. \tag{85}$$

One virtue of using η rather than ζ is that the pole at 1 has been removed. The other is that we have access to the alternating series acceleration methods of Section 4.4.4. We shall discuss further this below.

4.4.4 An eta-function approach to $\mathrm{Li}_s\left(\exp(i\theta)\right)$

There is another approach given in [22, Section 8.3] to computing $\mathrm{Li}_s(z), \mathrm{Li}_s\left(\exp(i\theta)\right)$, with applications especially to *alternating* MTW sums. This is and attractive, compact series, valid now for $|\log z| < \pi$,

$$\mathrm{Li}_s(-z) \;=\; -\sum_{m\geq 0}\eta(s-m)\frac{\log^m z}{m!}\ , \tag{86}$$

where now no poles need be avoided and so for $|\log z| < \pi$, and $d = 1, 2, \ldots$

$$\mathrm{Li}_s^{(d)}(-z) \;=\; -\sum_{m\geq 0}\eta^{(d)}(s-m)\frac{\log^m z}{m!}\ . \tag{87}$$

This is especially neat on the unit circle:

$$\mathrm{Li}_s^{(d)}\left(e^{i(\theta+\pi)}\right) \;=\; -\sum_{m\geq 0}\eta^{(d)}(s-m)\frac{(i\theta)^m}{m!}\ . \tag{88}$$

Alternatively, we have attractive Clausen formulas such as

$$\mathrm{Cl}_2^{(d)}(\pi-\theta) = \sum_{m\geq 0} \eta^{(d)}(1-2m)\frac{\theta^{2m+1}}{(2m+1)!}, \tag{89}$$

valid for $|\theta| < \pi$. For convenience we list that $\eta'(1) = \gamma \log 2 - \frac{1}{2}\log^2 2$ and $\eta^{(2)}(1) = \frac{1}{2}\left(\zeta(2)\log 2 + \zeta'(2)\right)$.

We note that if $\tau = \theta + \pi$ with $|\theta| < \pi$ then

$$\mathrm{Li}_{s_1}^{(d_1)}\left(-e^{i\theta}\right) = \mathrm{Li}_{s_1}^{(d_1)}\left(e^{i\tau}\right), \quad \mathrm{Li}_{s_2}^{(d_2)}\left(-e^{-i\theta}\right) = \mathrm{Li}_{s_2}^{(d_2)}\left(e^{i(-\pi-\theta)}\right) = \mathrm{Li}_{s_2}^{(d_2)}\left(e^{-i\tau}\right),$$

while $0 < \tau < 2\pi$.

It is not clear whether this relatively simple eta-series is applicable directly to compute general ω-values as in (5) using (88). One difficulty with such an approach is that convergence is very slow near an endpoint $|\log z| \sim \pi$; note that such z values challenge the radius of convergence of (86), while by contrast the more recondite series (61) enjoys a comfortably wider radius. In any case, the eta-series is certainly of interest for quadrature on alternating MTW sums which we do not cover in the present treatment.

One final topic we mention is how best to efficiently perform quadrature calculations of the sort indicated, for instance, for the $\mathcal{U}$ constants (7). Since the integrands in (7) are typically rather badly behaved, we recommend the tanh-sinh quadrature algorithm, which is remarkably insensitive to singularities at endpoints of the interval of integration.

4.5 Tanh-sinh quadrature

Given $h > 0$, the tanh-sinh quadrature scheme approximates the integral of a function $f(x)$ on $(-1, 1)$ as

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\,\mathrm{d}t \;\approx\; h \sum_{j=-N}^{N} w_j f(x_j), \tag{90}$$

where the abscissas x_j and weights w_j are given by

$$\begin{aligned} x_j &= g(hj) = \tanh\left(\pi/2 \cdot \sinh(hj)\right) \\ w_j &= g'(hj) = \pi/2 \cdot \cosh(hj) / \cosh\left(\pi/2 \cdot \sinh(hj)\right)^2, \end{aligned} \tag{91}$$

and where N is chosen large enough that terms of the summation beyond N (positive or negative) are smaller in absolute value than the "epsilon" of the numeric precision being used. Note that the abscissas x_j and weights w_j can be precomputed, and then applied to any number of quadrature calculations. For many integrand functions, including those indicated in (7), reducing h by half in (90) and (91) roughly doubles the number of correct digits in the approximation, provided the calculations are done to a precision level at least that desired for the final result. Full details are given in [9].

With regards to the $\mathcal{U}$ constant calculations, it suffices to perform the integral from 0 to π, then divide by π, rather than integrating to 2π, provided we integrate with the real part of the integrand function. It is also important to note that since one typically computes numerous different $\mathcal{U}(m, n, p, q)$ for different values of m, n, p and q, it is much faster to precompute, in an initialization step, the polylog functions and polylog derivative functions (sans the exponents) at each of the tanh-sinh abscissa points x_j. In this way, during an actual quadrature calculation, the evaluation of the integrand in (7) merely consists of table look-ups and a few multiplications for each function evaluation. In our implementations, quadrature calculations were accelerated by a factor of over 1000 by this expedient.

5 PART II. More recondite MTW interrelations

We now return to our objects of central interest.

5.1 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 7 (Reduction of classical MTW derivatives [5])**.** *Let nonnegative integers a, b, c and r, s, t be given. Set $N := r+s+t$. Then for $\delta := \omega_{a,b,c}$ we have*

$$\delta(r,s,t) = \sum_{i=1}^{r} \binom{r+s-i-1}{s-1} \delta\left(i, 0, N-i\right) + \sum_{i=1}^{s} \binom{r+s-i-1}{r-1} \delta\left(0, i, N-i\right). \tag{92}$$

In the case that $\delta = \omega$ this shows that each classical MTW value is a finite positive integer combination of MZVs.

Proof. 1. For non-negative integers r, s, t, v, with $r+s+t = v$, and v fixed, we induct on s. Both sides satisfy the same recursion:

$$d(r,s,t-1) = d(r-1,s,t) + d(r,s-1,t) \tag{93}$$

and the same initial conditions ($r+s = 1$).

Proof. 2. Alternatively, note that the recurrence produces terms of the same weight, N. We will keep the weight N fixed and just write $d(a,b)$ for $d(a,b,N-a-b)$.

By applying the recurrence (93) to $d(r,s)$ repeatedly until one of the variables r,s reaches 0, one ends up with summands of the form $d(k,0)$ or $d(0,k)$. As the problem is symmetric, we focus on the multiplicity with which $d(k,0)$ occurs. Note that, $d(k,0)$ is obtained from (93) if and only if one previously had $d(k,1)$. Thus, the multiplicity of $d(k,0)$ is the number of zig-zag paths from $(k,1)$ to (r,s) in which each step of a path adds either $(1,0)$ or $(0,1)$.

The number of such paths is given by

$$\binom{(r-k)+(s-1)}{s-1} = \binom{r+s-k-1}{s-1}.$$

This again proves the claim. ∎

Of course (92) holds for any δ satisfying the recursion (without being restricted to partial derivatives). This argument generalizes to arbitrary depth. We illustrate the next case from which the general case will be obvious if a tad inelegant.

Theorem 8 (Partial reduction of $\omega(q,r,s\mid t)$)**.** *For non-negative integer q,r,s,t, assume that $d(q,r,s,t)$ satisfies the recurrence*

$$d(q,r,s,t)=d(q-1,r,s,t+1)+d(q,r-1,s,t+1)+d(r,s-1,t+1)\,. \tag{94}$$

Let $N:=q+r+s+t$. Then

$$\begin{aligned}
d(q,r,s,t) &= \sum_{k=1}^{r}\sum_{j=1}^{s}\binom{N-t-k-j-1}{q-1,r-k,s-j}d(0,k,j,N-k-j)\\
&+ \sum_{k=1}^{q}\sum_{j=1}^{s}\binom{N-t-k-j-1}{q-k,r-1,s-j}d(k,0,j,N-k-j)\\
&+ \sum_{k=1}^{q}\sum_{j=1}^{r}\binom{N-t-k-j-1}{q-k,r-j,s-1}d(k,j,0,N-k-j)\,.
\end{aligned}$$

Example 8 (Values of δ)**.** Herein we use the shorthand notation

$$\omega_{a,b,c}(r,s,t):=\omega\begin{pmatrix} r\ ,\ s & \mid & t\\ a\ ,\ b & \mid & c\end{pmatrix}.$$

The techniques in [22] provide:

$$\omega_{1,1,0}(1,0,3) = 0.07233828360935031113948057244763953352659776102642...$$

$$\omega_{1,1,0}(2,0,2) = 0.29482179736664239559157187114891977101838854886937848122804...$$

$$\omega_{1,1,0}(1,1,2) = 0.14467656721870062227896114489527906705319552205284127904072...$$

while

$$\omega_{1,0,1}(1,0,3) = 0.14042163138773371925054281123123563768136197000104827665935...$$

$$\omega_{1,0,1}(2,0,2) = 0.40696928390140268694035563517591371639834128770661373815447...$$

$$\omega_{1,0,1}(1,1,2) = 0.43097253394888316942248176511038963971077201581912157523909...$$

and

$$\omega_{0,1,1}(2,1,1) = 3.00297121355668005079211509351534225995879828374320045987 9...$$

We note that $\omega_{1,1,0}(1,1,2) = 2\,\omega_{1,1,0}(1,0,3)$ and $\omega_{1,0,1}(1,0,3) + \omega_{1,0,1}(0,1,3) - \omega_{1,0,1}(1,1,2)$

$$= 0.140421631387733719247 + 0.290550902561149450012 - 0.430972533948883169420$$

$$= 0.0000000000000000000...,$$

both in accord with Theorem 7. We note also that PSLQ run on the above data predicts that

$$\zeta''(4) \stackrel{?}{=} 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2) - 2\,\omega_{1,0,1}(2,0,2), \tag{95}$$

which discovery also validates the effectiveness of our high-precision techniques. $\Diamond$

From (95) it is clear that much less trivial derivative relations exist within $\mathcal{D}$ than can be found within $\mathcal{D}_1$. Indeed, as noted in (120)

$$\mathcal{U}(1,1,1,1) = \omega \begin{pmatrix} 1 & | & 1 \\ 1 & | & 1 \end{pmatrix} = \zeta''(2). \tag{96}$$

More generally, with $\zeta_{a,b}$ denoting partial derivatives, it is immediate that

$$\omega \begin{pmatrix} s, & 0\,| & t \\ a, & 0\,| & b \end{pmatrix} = \zeta_{a,b}(t,s) \tag{97}$$

$$\omega \begin{pmatrix} s, & t\,| & 0 \\ a, & b\,| & 0 \end{pmatrix} = \zeta^{(a)}(s)\,\zeta^{(b)}(t). \tag{98}$$

We may now prove (95):

Proposition 1.

$$\zeta''(4) = 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2) - 2\,\omega_{1,0,1}(2,0,2). \tag{99}$$

Proof. First note that by (98)

$$\omega_{1,1,0}(2,2,0) = \zeta^{'}(2)^2.$$

Next the MZV reflection formula $\zeta(s,t) + \zeta(t,s) = \zeta(s)\zeta(t) - \zeta(s+t)$, see [10], valid for real $s,t > 1$ yields $\zeta_{1,1}(s,t) + \zeta_{1,1}(t,s) = \zeta'(s)\zeta'(t) - \zeta^{(2)}(s+t)$. Hence

$$2\omega_{1,0,1}(2,0,2) = 2\zeta_{1,1}(2,2) = \zeta'(2)^2 - \zeta''(4)$$

where the first equality follows from (97). Since $\omega_{1,1,0}(2,0,2) = 2\omega_{1,0,1}(2,1,1)$ by Theorem 7, our desired formula (99) is

$$\zeta^{''}(4) + 2\,\omega_{1,0,1}(2,0,2) = 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2), \tag{100}$$

which is equivalent to

$$\zeta^{'}(2)^2 = \omega_{1,1,0}(2,2,0) = 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2). \tag{101}$$

The final equality is another easy case of Theorem 7. $\square$

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

In general we deduce from (2), by a now familiar partial fraction argument that since $\sum t_k = \sum s_j$ we have

Theorem 9 (Relations for general ω).

$$\sum_{k=1}^{N} \omega \begin{pmatrix} s_1, \ldots, s_M & | & t_1, \ldots, t_{k-1}, t_k - 1, t_{k+1}, \ldots, t_N \\ d_1, \ldots, d_M & | & e_1, \ldots e_N \end{pmatrix}$$

$$= \sum_{j=1}^{M} \omega \begin{pmatrix} s_1, \ldots, s_{j-1}, s_j - 1, s_{j+1}, \ldots, s_M & | & t_1, \ldots, t_N \\ d_1, \ldots, d_M & | & e_1, \ldots e_N \end{pmatrix}. \tag{102}$$

When $N = 1$ and $M = 2$ this is precisely (93). For general M and $N = 1$ there is a result like Theorem 8.

For $N > 1$ we will be able to deduce relations but have found no such reduction.

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

When $N = 1$ it is possible to use Theorem 9 to show that every MTW value (without 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 detail this algorithmically for $M = 3$ before presenting a general theorem.

1. Use (102) to recursively write $\omega(q, r, s \mid t)$ as a superposition of terms $\omega(a, b, 0 \mid c)$ (appealing to symmetry reduces the number of terms): first

$$\omega(q, r, s \mid t) = \omega(q-1, r, s \mid t+1) + \omega(q, r-1, s \mid t+1) + \omega(q, r, s-1 \mid t+1). \tag{103}$$

   We run this at $t \mapsto t+1$ until one of the RHS variable reaches zero.

2. Define

$$\kappa(a, b \mid t, u) := \sum_{n,m,k>0} \frac{1}{n^a m^b (n+m)^t (n+m+k)^u}, \tag{104}$$

3. Observe that

$$\kappa(a, b \mid 0, c) = \omega(a, b, 0 \mid c) \quad \text{while} \quad \kappa(a, 0 \mid b, c) = \zeta(c, b, a).$$

4. Now, using partial fractions as before, yields

$$\kappa(a,b \mid t,u) = \kappa(a-1,b \mid t+1,u) + \kappa(a,b-1 \mid t+1,u). \tag{105}$$

5. Then used recursively, (105) writes each $\omega(a,b,0 \mid c)$ as a superposition of $\zeta(c,b,a)$ as required because we again let $t \mapsto t+1$ and terminate when one of the a,b variables reaches zero.

Example 9 (An implementation)**.** The precise superposition formula is achieved by combining Theorem 7 and Theorem 8. Implemented in *Maple* this becomes:

```
W3:=proc (q, r, s, t) if q = 0 then kappa(r, s, 0, t) elif r = 0 then
 kappa(q, s, 0, t) elif s = 0 then kappa(q, r, 0, t)
         else W3(q-1, r, s, t+1)+W3(q, r-1, s, t+1)+W3(q, r, s-1, t+1)
         end if: end proc:


kappa:=proc(q,r,s,t) ;if q=0  then zeta(t,s,r) elif r=0 then zeta(t,s,q)
        else  kappa(q-1,r,s+1,t)+kappa(q,r-1,s+1,t) fi;end:
>W3(1,1,1,1);
                        6 zeta(2, 1, 1) = 6 Zeta(4)
>W3(3,2,1,1);
   12*Zeta(4, 2, 1)+6*Zeta(4, 1, 2)+18*Zeta(5, 1, 1)+4*Zeta(3, 2, 2)+8*Zeta(3, 3, 1)+2*Zeta(3, 1, 3)
   +3*Zeta(2, 3, 2)+6*Zeta(2, 4, 1)+Zeta(2, 2, 3)
```

Given efficient computations of the final MZVs, this is a very rapid process for numerical computation of reasonable depth and weight MTWs with $N = 1$. $\Diamond$

With much the same argument this works cleanly for all M. Each time we get another zero we get a recursion in one less variable until we remove all except one of the single variables. Thus, we derive:

Theorem 10 (Complete reduction of $\omega(a_1, a_2, \ldots, a_M \mid b)$)**.** *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.

Proof. For (a), let us define $N_j := n_1 + n_2 + \cdots n_j$ and set

$$\kappa(a_1, \dots a_n \mid b_1, \dots b_n) := \sum_{n_i > 0} \frac{1}{\prod_{i=1}^n n_i^{a_i} \prod_{j=1}^n N_j^{b_j}}, \tag{106}$$

for positive integers a_i and non negative b_j (with b_n large enough to assure convergence). Thence $\kappa(a_1, \dots a_n \mid b_1) = \omega(a_1, \dots a_n \mid b_1)$. Noting that κ is symmetric in the a_i we denote $\overrightarrow{a}$ to be the non-increasing rearrangement of $\overline{a} := (a_1, a_2, \cdots, a_n)$. Let k be the largest index of a non-zero element in $\overrightarrow{a}$. Using the partial fraction above, we have

$$\kappa(\overline{a} \mid \overline{b}) = \kappa(\overrightarrow{a} \mid \overline{b}) = \sum_{j=1}^{k} \kappa(\overrightarrow{a} - e_j, \mid \overline{b} + e_k).$$

We repeat this step until there are only $k-1$ non-zero entries. Each step leaves the weight of the sum invariant. Continuing this process (observing that the repeated rearrangements leave the N_j terms invariant) we arrive at a superposition of sums of the form

$$\kappa(\overrightarrow{0} \mid \overline{b}) = \zeta(b_n, b_{n-1}, \dots, b_1).$$

Moreover, the process assures that each variable is reduced to zero and so each final $b_j > 0$. In particular, we may start with κ such that each $a_i > 0$ and $b_j = 0$ except for $j = n$. This captures all our ω sums and other intermediate structures.

Part (b) follows from recent results in the MZV literature [36]. □

Tsimura [37] provides a reduction theorem for exactly our MTWs with $N = 1$ to lower weight MTWs. In light of Theorem 10, this result is subsumed by his earlier paper [36]. As we discovered later, Theorem 10 was recently proven very neatly by explicit combinatorial methods in [19], which do not lend themselves to our algorithmic needs.

5.4 Degenerate MTW derivatives with zero numerator values

In Theorem 10 we make no such assertion about derivative values—our zero value may still have a log term in the corresponding variable—nor about the case with $N \geq 2$. For example, it appears unlikely that

$$\omega \left(\begin{array}{cc|c} 1 \, , & 0 & 2 \\ 0 \, , & 1 & 0 \end{array} \right) = \sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^{n-1} \frac{\log(n-m)}{m} \tag{107}$$

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

$$\omega \left(\begin{array}{cc|c} 0 \, , & 0 & s \\ 0 \, , & 1 & 0 \end{array} \right) = -\sum_{n=2}^{\infty} \frac{\log \Gamma(n)}{n^s}. \tag{108}$$

We observe that such ω values with terms of order zero cannot be computed directly from the integral form of (5) without special attention to convergence at the singularities. Instead we may recast such *degenerate* derivative cases as:

$$\omega \left(\begin{array}{cc|c} q \, , & r & s \\ 0 \, , & 1 & 0 \end{array} \right) = \frac{1}{\Gamma(s)} \int_0^{\infty} x^{s-1} \mathrm{Li}_q(e^{-x}) \, \mathrm{Li}_r^{(1)}(e^{-x}) \, \mathrm{d}x. \tag{109}$$

Though we have deemed it unlikely that MTW derivatives can be cast as finite superpositions of MZV derivatives, it is yet possible to go some distance in establishing some (non finitary) relations. Consider the development

$$\omega\begin{pmatrix} r\ ,\ 0 & \mid & s \\ 0\ ,\ 1 & \mid & 0 \end{pmatrix} = -\sum_{m,n\geq 1}\frac{1}{m^r}\log n\frac{1}{(m+n)^s} \tag{110}$$

$$= -\sum_{N\geq 1}\frac{1}{N^s}\sum_{M=1}^{N-1}\frac{\log(N-M)}{M^r}$$

$$= \zeta^{(1,0)}(s,r)\ +\ \sum_{k\geq 1}\frac{1}{k}\zeta(s+k,r-k).$$

Here, $\zeta^{(1,0)}(s,r)$ is the first parametric derivative $\partial\zeta(s,r)/\partial s$. What is unsatisfactory about in this last expression is that the k-sum is not a finite superposition—although it *does* converge, as is not hard to show in the following way.

For given r, t turns out that *only finitely many* $\zeta(s+k,r-k)$ *cannot be given closed form.* Indeed,

$$\sum_{k\geq 1}\frac{1}{k}\zeta(s+k,r-k)\ =\ \sum_{k=1}^{r}\frac{1}{k}\zeta(s+k,r-k)\ +\ T_r, \tag{111}$$

where the MZV summands on the right here may well have no closed form, but T_r is

$$T_r = \sum_{k>r}\frac{1}{k}\sum_{N\geq 1}\frac{1}{N^{s+k}}\sum_{m=1}^{N-1}M^{k-r},$$

with the M-sum being expressible in classical style as a sum of powers of N. Asymptotically, the M-sum is thus $O(N^{k-r}/(k-r))$ so that the tail T_r always converges.

Explicitly, in terms of Bernoulli numbers,

$$T_r = \sum_{k>r} \frac{1}{k} \frac{1}{k-r+1} \sum_{j=1}^{k-r+1} \binom{k-r+1}{j} B_{k-r+1-j}\, \zeta(s+k-j). \tag{112}$$

All of this shows that the MTW derivative in question can be expressed as

(MZV derivative) + (finite superposition of MZV's) + (rational zeta series).

Example 10. Returning to our example (108) with power $r = 0$, we have the decomposition

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

$$= \zeta'(s-1) - \zeta'(s) + \sum_{k\geq 1} \frac{1}{k}\, \zeta(s+k, -k),$$

where, as we have see, the MZV's occurring in the tail, while infinite in number, each have a closed form in terms of Riemann zetas alone. Thus, it is not out of the question that this final sum might yet be reducible. $\square$

6 MTW resolution of the log-gamma problem

As a larger example of our interest in such MTW sums we shall show that the subensemble $\mathcal{D}_1$ from Section 2.1 completely resolves of the log-gamma integral problem [5]—in that every one of our log-gamma integrals $\mathcal{LG}_n$ lies in a specific algebra.

6.1 Log-gamma representation

We start, as in [5] with the Kummer series, see [2, p. 28], or [30, (15) p. 201]:

$$\begin{aligned}\log\Gamma(x) - \frac{1}{2}\log(2\pi) &= -\frac{1}{2}\log\left(2\sin(\pi x)\right) + \frac{1}{2}(1-2x)\left(\gamma + \log(2\pi)\right) \\ &\quad + \frac{1}{\pi}\sum_{k=2}^{\infty}\frac{\log k}{k}\sin(2\pi k x)\end{aligned} \tag{113}$$

for $0 < x < 1$. But with a view toward polylogarithm representations, this can be satisfactorily written as:

$$\log\Gamma\left(\frac{z}{2\pi}\right) - \frac{1}{2}\log 2\pi \;=\; A\,\mathrm{Li}_1(e^{iz}) + B\,\mathrm{Li}_1(e^{-iz}) + C\,\mathrm{Li}_1^{(1)}(e^{iz}) + D\,\mathrm{Li}_1^{(1)}(e^{-iz}), \tag{114}$$

where the absolute constants are

$$A := \frac{1}{4} + \frac{1}{2\pi i}(\gamma + \log 2\pi),\;\; C := -\frac{1}{2\pi i},\;\; B := A^*,\;\; D := C^*. \tag{115}$$

Here $'*'$ denotes the complex conjugate.

We define a vector space $\mathcal{V}_1$ whose basis is the subensemble $\mathcal{D}_1$, with coefficients generated by the rationals $\mathcal{Q}$ together with a certain four fundamental constants:

$$c_i \;\in\; \left\{\mathcal{Q} \;\cup\; \left\{\pi, \frac{1}{\pi}, \gamma, g := \log 2\pi\right\}\right\}.$$

Specifically,

$$\mathcal{V}_1 \;:=\; \left\{\sum c_i\omega_i \;:\; \omega_i \in \mathcal{D}_1\right\},$$

where any sum therein is finite.

These observations lead to a resolution of the Eulerian log-gamma problem, which is to request to evaluate integrals

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

As foreshadowed in [5]:

Theorem 11. *For every integer $n \geq 0$, the n-th log-gamma integral can be resolved in the sense that $\mathcal{LG}_n \;\in\; \mathcal{V}_1$.* (The proof exhibits an explicit form for the requisite superposition $\sum c_i\omega_i$ for any n.)

Proof. By induction. It is enough to show that generally

$$\mathcal{G}_n \;:=\; \int_0^1 \left(\log\Gamma(z) \;-\frac{g}{2}\right)^n \,dz \tag{116}$$

is in $\mathcal{V}_1$, because it is a classic Eulerian result that $\mathcal{LG}_1 = \frac{g}{2}$ (i.e. $G_1 = 0$), so that for $n > 1$ we may use recursion in the ring to resolve $\mathcal{LG}_n$. By formula (114), we write $\mathcal{G}_n$ as

$$\mathcal{G}_n \;:= n! \sum_{a+b+c+d=n} \frac{A^aB^bC^cD^d}{a!b!c!d!}\mathcal{U}(a+c, b+d, c, d),$$

where $\mathcal{U}$ has been defined by (7). This finite sum for G_n is in the vector space $\mathcal{V}_1$. $\square$

Example 11 (Examples of $\mathcal{G}$)**.** Some examples of the proof details are instructive at this juncture. We have, recalling $g := \log 2\pi$, the following:

For $n = 1$**,** we have Euler's evaluation [5]

$$\mathcal{G}_1 = \int_0^1 \left(\log\Gamma(z) - \frac{g}{2}\right) dz = 0. \tag{117}$$

For $n = 2$**,** so that the relevant generators from subensemble $\mathcal{D}_1$ have $a+b+c+d = 2$, and consistent with previous developments [1, 5], we can extract an algebra superposition for $\mathcal{LG}_2$ via

$$\begin{aligned}\mathcal{G}_2 &= \int_0^1 \left(\log\Gamma(z) - \frac{g}{2}\right)^2 dz \qquad (118)\\ &= \frac{(4(g+\gamma)^2+\pi^2)}{8\pi^2}\mathcal{U}(1,1,0,0) - \frac{(2g+2\gamma)}{4\pi^2}(\mathcal{U}(1,1,0,1)\\ &\quad +\mathcal{U}(1,1,1,0)) + \frac{\mathcal{U}(1,1,1,1)}{2\pi^2}. \qquad (119)\end{aligned}$$

Since $\mathcal{U}(1,1,0,0) = \zeta(2)$, while $\mathcal{U}(1,1,0,1) = \mathcal{U}(1,1,1,0) = \zeta'(2)$, and $\mathcal{U}(1,1,1,1) = \zeta''(2)$, this decodes as

$$\begin{aligned}\mathcal{LG}_2 &= \frac{1}{4}\log^2(2\pi) + \frac{1}{48}\pi^2 + \frac{1}{12}(\gamma+\log(2\pi))^2 - \frac{1}{\pi^2}(\gamma+\log(2\pi))\,\zeta'(2)\\ &\quad + \frac{1}{2\pi^2}\zeta''(2).\end{aligned} \tag{120}$$

For $n = a+b+c+d = 3$ we obtain (in the following we set $h := \gamma + \log 2\pi$)

$$\mathcal{G}_3 = \int_0^1 \left(\log\Gamma(z) - \frac{g}{2}\right)^3 dz \tag{121}$$

$$= \frac{3\,(4h^2+\pi^2)}{32\pi^2}\mathcal{U}(2,1,0,0) - \frac{3h}{4\pi^2}\mathcal{U}(2,1,0,1) + \frac{3}{4\pi^2}\mathcal{U}(2,1,1,1) - \frac{3}{8\pi^2}\mathcal{U}(2,1,2,0). \tag{122}$$

For $n = a+b+c+d = 4$ we obtain

$$\mathcal{G}_4 = \int_0^1 \left(\log\Gamma(z) - \frac{g}{2}\right)^4 dz \tag{123}$$

$$\begin{aligned}
&= \frac{(\pi^4-16h^4)\,\mathcal{U}(3,1,0,0)}{32\pi^4} + \frac{(4h^3-3\pi^2h)\,\mathcal{U}(3,1,0,1)}{8\pi^4} \\
&+ \frac{3\,(4h^2+\pi^2)^2\,\mathcal{U}(2,2,0,0)}{128\pi^4} - \frac{3h\,(4h^2+\pi^2)\,\mathcal{U}(2,2,0,1)}{16\pi^4} \\
&- \frac{3h\,(4h^2+\pi^2)\,\mathcal{U}(2,2,1,0)}{16\pi^4} + \frac{3\,(4h^2+\pi^2)\,\mathcal{U}(2,2,1,1)}{8\pi^4} \\
&+ \frac{3h\,(4h^2+\pi^2)\,\mathcal{U}(3,1,1,0)}{8\pi^4} - \frac{3\,(4h^2+\pi^2)\,\mathcal{U}(3,1,2,0)}{8\pi^4} \\
&- \frac{3\,(\pi^2-4h^2)\,\mathcal{U}(2,2,0,2)}{32\pi^4} - \frac{3\,(\pi^2-4h^2)\,\mathcal{U}(2,2,2,0)}{32\pi^4} \\
&+ \frac{3\,(\pi^2-4h^2)\,\mathcal{U}(3,1,1,1)}{8\pi^4} - \frac{3h\mathcal{U}(2,2,1,2)}{4\pi^4} \\
&- \frac{3h\mathcal{U}(2,2,2,1)}{4\pi^4} + \frac{3h\mathcal{U}(3,1,2,1)}{2\pi^4} + \frac{h\mathcal{U}(3,1,3,0)}{2\pi^4} \\
&+ \frac{3\mathcal{U}(2,2,2,2)}{8\pi^4} - \frac{\mathcal{U}(3,1,3,1)}{2\pi^4}.
\end{aligned} \tag{124}$$

For $n = a + b + c + d = 5$, we can extract the previously unresolved $\mathcal{LG}_5$ from

$$\mathcal{G}_5 = \int_0^1 \left(\log\Gamma(z) \; - \frac{g}{2}\right)^5 \, dz \tag{125}$$

$$\begin{aligned} &= \frac{5\left(4h^2+\pi^2\right)^2}{256\pi^4}\mathcal{U}(3,2,0,0) - \frac{5h\left(4h^2+\pi^2\right)}{16\pi^4}\mathcal{U}(3,2,0,1) \\ &+ \frac{15\left(4h^2+\pi^2\right)}{32\pi^4}\mathcal{U}(3,2,1,1) - \frac{15\left(4h^2+\pi^2\right)}{64\pi^4}\mathcal{U}(3,2,2,0) \\ &+ \frac{5\left(\pi^2-12h^2\right)\left(4h^2+\pi^2\right)}{512\pi^4}\mathcal{U}(4,1,0,0) + \frac{5h\left(4h^2+\pi^2\right)}{16\pi^4}\mathcal{U}(4,1,1,0) \\ &- \frac{15\left(4h^2+\pi^2\right)}{64\pi^4}\mathcal{U}(4,1,2,0) + \frac{5\left(12h^2-\pi^2\right)}{64\pi^4}\mathcal{U}(3,2,0,2) - \frac{15h}{8\pi^4}\mathcal{U}(3,2,1,2) \\ &+ \frac{5h}{8\pi^4}\mathcal{U}(3,2,3,0) + \frac{5\left(\pi^2-12h^2\right)}{32\pi^4}\mathcal{U}(4,1,1,1) + \frac{15h}{8\pi^4}\mathcal{U}(4,1,2,1) \\ &+ \frac{5h\left(4h^2-\pi^2\right)}{32\pi^4}\mathcal{U}(4,1,0,1) + \frac{15}{16\pi^4}\mathcal{U}(3,2,2,2) - \frac{5}{8\pi^4}\mathcal{U}(3,2,3,1) \\ &- \frac{5}{8\pi^4}\mathcal{U}(4,1,3,1) + \frac{5}{32\pi^4}\mathcal{U}(4,1,4,0). \end{aligned} \tag{126}$$

For both $n = 2$ and $n = 3$ these evaluations lead to those previously published in [5].

To clarify the notation in these recondite expressions, we state two example terms—namely the last $\mathcal{U}$-value above for $\mathcal{G}_5$, which is

$$\mathcal{U}(4,1,4,0) \;=\; \omega\begin{pmatrix} 1,1,1,1 & | & 1 \\ 1,1,1,1 & | & 0 \end{pmatrix} \;=\; \sum_{m,n,p,q} \frac{\log m\,\log n\,\log p\,\log q}{m\,n\,p\,q\,(m+n+p+q)}. \tag{127}$$

and the double MTW sum:

$$\mathcal{U}(3,2,3,0) \;=\; \omega\begin{pmatrix} 1,1,1 & | & 1,1 \\ 1,1,1 & | & 0,0 \end{pmatrix} \;=\; \sum_{m,n,p,q}{}' \frac{\log m\,\log n\,\log p}{m\,n\,p\,q\,(m+n+p-q)}. \tag{128}$$

Here the '$'$' indicates we avoid the poles. It is a triumph of the integral representations that very slowly convergent sums such as (127) and (128) (of weight nine and eight respectively) can be calculated to extreme precision in short time. $\Diamond$

Remark 3. In all the examples above $\pi^{n-1}\mathcal{L}\mathcal{G}_N$ is realized with no occurrence of $1/\pi$; with more care it should be possible to adduce this in the proof of Theorem 11. $\Diamond$

6.2 An exponential generating function for the $\mathcal{LG}_n$

To conclude this analysis, we yet again turn to generating functions. Let us define:

$$\mathcal{Y}(x) := \sum_{n\geq 0} \mathcal{LG}_n \frac{x^n}{n!} \;=\; \int_0^1 \Gamma^x(1-t)\,\mathrm{d}t. \tag{129}$$

Now, from the exponential-series form for Γ given in (23), it follows quickly that the general log-gamma integral is expressible as follows

Theorem 12. *For $n = 1, 2, \ldots$ we have the infinite sum representation*

$$\mathcal{LG}_n \;=\; \sum_{m_1,\ldots,m_n\geq 1} \frac{\zeta^*(m_1)\,\zeta^*(m_2)\cdots\zeta^*(m_n)}{m_1 m_2\cdots m_n(m_1+\cdots+m_n+1)}, \tag{130}$$

where $\zeta^*(1) := \gamma$ and $\zeta^*(n) := \zeta(n)$ for $n \geq 2$.

In particular, the Euler's evaluation of $\mathcal{LG}_1$ leads to

$$\log\sqrt{2\pi} \;=\; \sum_{m\geq 1} \frac{\zeta^*(m)}{m(m+1)}$$

$$= \frac{1}{2} \;+\; \gamma \;+\; \sum_{m\geq 2} \frac{\zeta(m)-1}{m(m+1)},$$

a rapidly convergent rational eta-series. It is fascinating — and not completely understood — how the higher $\mathcal{LG}_n$ can be finite superpositions of *derivative* MTWs, as we know, and yet for any index n these log-gamma integrals as infinite sums engage only the ζ-function convolutions as above.

7 Numerical experiments

In an effort both to check our theory and evaluations above, and also to further explore the space of the constants and functions being analyzed, we performed several numerical computations.

7.1 Computations of the $\mathcal{G}$ constants

In our first computation, we computed $\mathcal{G}(2)$, $\mathcal{G}(3)$, $\mathcal{G}(4)$ and $\mathcal{G}(5)$ to 400-digit precision, using *Mathematica* and the formulas (118), (121), (123) and (125). Then we separately computed these constants using formulas (119), (122), (124) and (126). This second set of computations was performed with a combination of the ARPREC arbitrary precision software [8] and our implementation of the tanh-sinh quadrature algorithm (90) to compute the numerous $\mathcal{U}$ constants that appear in formulas (119), (122), (124) and (126). We employed formulas (51), (52), (59) and (61) to evaluate the underlying polylog and polylog derivatives; and formulas (62), (63), (65), (66) and (67) to evaluate the underlying zeta and zeta derivatives.

The results of these two sets of calculations matched to 400-digit accuracy. Here are our 400-digit values for $\mathcal{G}_n$, $2 \leq n \leq 5$:

```
G(2) =
1.02186905598520665379766897429270227225728935347049021404932007954291
4822812230316346019965407178139635519941059164807745247326926309995731
3997512255380295930794029004152862173913702886050064547476514918837221
7346957031918547469003562890989649716395646738011214999052870333851453
2595110642589149987197987780589087047152829297434202593887423392443879
356534311066730513877700759535491416157266885504624
```

```
G(3) =

2.14728842088481720475269216366752854640150302596977765026060123588067

7893912441157610058141066676835926293341902057894078837376205988048214

8963659830320543721667041466157167523983756252527974024505366516994405

7596718898020238066116241903185583841968941772265741033501952971299841

8570206825260401573989607602934975337547900377338567431714882998611155

557913683043153310887854877943542378021990121314709
```

```
G(4) =

9.60602585239573084465874355932859101433487909011737193052140866424016

8543744548145772529154110491198133159166578474713719703476791766191772

2704888404405652032031452183897414363176292592388705963322455027839376

2795846069975498418148001664977372622808879413712730474756056358114225

4072014549038507972369233469175958231773693152249524436176693770966660

496333905460471600762705190138485178869197636008376
```

```
G(5) =

47.4443724960735762605374696417757945376635206983622256690323974264225

4997279623094143877934035405384936621025013904885767766916639053013698

5604936790731080045401985995190510803727972851864406009936892475769746

5242705758870675007514112686748506926573143012447629869603635313065767

0858057703878739201258725226176055659160950274041647798759870204366752

333418078619509916338886221328957064336634718497078
```

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

In a subsequent calculation, we computed, to 3100-digit precision, all of the $\mathcal{U}$ constants in the class $\mathcal{D}_1$ up to degree 10 (i.e., whose indices sum to 10 or less), according to the defining formula (7) and the rules given for $\mathcal{D}_1$ in Section 2.1. In particular, we calculated $\mathcal{U}(m, n, p, q)$ with $m, n \geq 1$, $m \geq n$, $m \geq p$, $n \geq q$, $m + n + p + q \leq 10$. Our computer program found that there are 149 constants in this class.

These computations, as above, were performed using the ARPREC arbitrary precision software [8] and the tanh-sinh quadrature algorithm (90), employing formulas (51), (52), (59) and (61) to evaluate the underlying polylog and polylog derivatives; and formulas (62), (63), (65), (66) and (67) to evaluate the underlying zeta and zeta derivatives.

We then searched among this set of numerical values for linear relations, using the multipair "PSLQ" integer relation algorithm [7], [13, pg. 230–234]. Our program first found the following relations, confirmed to over 3000-digit precision:

$$0 = \mathcal{U}(M, M, p, q) - \mathcal{U}(M, M, q, p), \tag{131}$$

for $M \in [1, 4]$ and $2M + p + q \in [2, 10]$, a total of 11 relations.

These relations are easy to establish, either by exchanging variables in the summation definition for $\mathcal{U}$, or by noting that when $m = n = M$, interchanging p and q in the integrand of (7) is equivalent to merely taking the conjugate of the integrand, which, since the integral is real, leaves the result unchanged. The fact that the programs uncover these simple symmetry relations gave us some measure of confidence that software was working properly.

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

$$
\begin{aligned}
0 &= 6\mathcal{U}(2,2,0,0) - 11\mathcal{U}(3,1,0,0) \\
0 &= 160\mathcal{U}(3,3,0,0) - 240\mathcal{U}(4,2,0,0) + 87\mathcal{U}(5,1,0,0) \\
0 &= 1680\mathcal{U}(4,4,0,0) - 2688\mathcal{U}(5,3,0,0) + 1344\mathcal{U}(6,2,0,0) - 389\mathcal{U}(7,1,0,0) \\
0 &= 32256\mathcal{U}(5,5,0,0) - 53760\mathcal{U}(6,4,0,0) + 30720\mathcal{U}(7,3,0,0) - 11520\mathcal{U}(8,2,0,0) \\
&\quad + 2557\mathcal{U}(9,1,0,0). \qquad (132)
\end{aligned}
$$

Upon completion of the final relation search, our PSLQ program reported an exclusion bound of 2.351×10^{19}. This means that if there is any integer linear relation among the set of 149 constants that is not listed above, then the Euclidean norm of the corresponding vector of integer 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).

The entire computation just described, 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, as well as 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 [9]) required 82074 seconds.

After initialization, the 149 quadrature calculations completed rather quickly (a total of 6894 seconds), as did the 16 PSLQ calculations (a total of 5760 seconds).

We observe that these relations can be established by using *Maple* to symbolically evaluate the righthand side of (25) as described in the second proof of Theorem 2 or as in Example 1. 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 (132). Likewise, the second relation is a consequence of the three evaluations:

$$\begin{aligned}
\mathcal{U}(3,3,0,0) &= \frac{963}{4}\,\zeta(6) + 36\,\zeta(3)^2 \\
\mathcal{U}(4,2,0,0) &= 204\,\zeta(6) + 24\,\zeta(3)^2 \\
\mathcal{U}(5,1,0,0) &= 120\,\zeta(6).
\end{aligned}$$

Similarly, the third relation in (132) follows from

$$\begin{aligned}
\mathcal{U}(4,4,0,0) &= 11103\,\zeta(8) + 2304\,\zeta(5)\,\zeta(3) + 576\,\zeta(3)^2\,\zeta(2) \\
\mathcal{U}(5,3,0,0) &= 10350\,\zeta(8) + 2160\,\zeta(5)\,\zeta(3) + 360\,\zeta(3)^2\,\zeta(2) \\
\mathcal{U}(6,2,0,0) &= 8280\,\zeta(8) + 1440\,\zeta(5)\,\zeta(3) \\
\mathcal{U}(7,1,0,0) &= 5040\,\zeta(8).
\end{aligned}$$

And so on.

7.3 A conjecture posited, then proven

From the equations in (132) we *conjectured* that (i) there is one such relation at each even weight— $4, 6, 8, \ldots$ — and none at odd weight, and (ii) that in each case $p = q = 0$. In other words, there appear to be no nontrivial relations between derivatives within the ensemble outside $\mathcal{D}_0$ but in $\mathcal{D}_1$. Any negative results must perforce be empirical as one cannot at the present prove things as ‘simple‘ as the irrationality of $\zeta(5)$.

Accordingly, we performed a second computation, this time using only 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 following additional relations:

$$
\begin{aligned}
0 &= 163451904\mathcal{U}(6,6,0,0) - 280203264\mathcal{U}(7,5,0,0) + 175127040\mathcal{U}(8,4,0,0) \\
&\quad - 77834240\mathcal{U}(9,3,0,0) + 23350272\mathcal{U}(10,2,0,0) - 4245819\mathcal{U}(11,1,0,0) \\
0 &= -35143680\mathcal{U}(7,7,0,0) + 61501440\mathcal{U}(8,6,0,0) - 41000960\mathcal{U}(9,5,0,0) \\
&\quad + 20500480\mathcal{U}(10,4,0,0) - 7454720\mathcal{U}(11,3,0,0) + 1863680\mathcal{U}(12,2,0,0) \\
&\quad - 286719\mathcal{U}(13,1,0,0) \\
0 &= 47668008960\mathcal{U}(8,8,0,0) - 84743127040\mathcal{U}(9,7,0,0) \\
&\quad + 59320188928\mathcal{U}(10,6,0,0) - 32356466688\mathcal{U}(11,5,0,0) \\
&\quad + 13481861120\mathcal{U}(12,4,0,0) - 4148264960\mathcal{U}(13,3,0,0) \\
&\quad + 888913920\mathcal{U}(14,2,0,0) - 118521871\mathcal{U}(15,1,0,0)
\end{aligned}
$$

and

$$
\begin{aligned}
0 \quad = \quad & -698880340787200\mathcal{U}(9,9,0,0) + 1257984613416960\mathcal{U}(10,8,0,0) \\
& -914897900666880\mathcal{U}(11,7,0,0) + 533690442055680\mathcal{U}(12,6,0,0) \\
& -246318665564160\mathcal{U}(13,5,0,0) + 87970951987200\mathcal{U}(14,4,0,0) \\
& -23458920529920\mathcal{U}(15,3,0,0) + 4398547599360\mathcal{U}(16,2,0,0) \\
& -517476186270\mathcal{U}(17,1,0,0) \\
0 \quad = \quad & -1479953674482483200\mathcal{U}(10,10,0,0) + 2690824862695424000\mathcal{U}(11,9,0,0) \\
& -2018118647021568000\mathcal{U}(12,8,0,0) + 1241919167397888000\mathcal{U}(13,7,0,0) \\
& -620959583698944000\mathcal{U}(14,6,0,0) + 248383833479577600\mathcal{U}(15,5,0,0) \\
& -77619947962368000\mathcal{U}(16,4,0,0) + 18263517167616000\mathcal{U}(17,3,0,0) \\
& -3043919527936000\mathcal{U}(18,2,0,0) + 320412581915500\mathcal{U}(19,1,0,0)
\end{aligned} \tag{133}
$$

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-mentioned relations, no other relations were found, with exclusion bounds of at least 2.481×10^{75}.

Remark 4. It is gratifying indeed that our computer facilities are both able to numerically discover such intriguing relations and to establish all instances obtained via symbolic processing. We have mentioned that the suggested conjecture (at least the even-weight part) has been proven as our Theorem 3; we repeat that 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 the results for $\mathcal{U}_s$ accessible. $\Diamond$

7.4 Computational notes

We should add that this exercise has underscored the need for additional research and development in the arena 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 on our own computer programs and the ARPREC arbitrary precision software in this study in part because we were unable to obtain the needed functionality in commercial software.

For instance, neither *Maple* nor *Mathematica* was able to numerically evaluate the $\mathcal{U}_1$ constants to high precision in reasonable run time, in part because of the challenge of computing polylog and polylog derivatives at complex arguments. The version of *Mathematica* that we were using was able to numerically evaluate $\partial \mathrm{Li}_s(z)/\partial s$ to high precision, which is required in (7), 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.

8 Future research directions

One modest research issue is further simplification of log-gamma integrals, say by reducing in some fashion the examples of Theorem 11. Note that we have optimally reduced $\mathcal{U}(M,N) := \mathcal{U}(M,N,0,0)$, in the form of explicit ζ-superpositions in a specific ring, and we have excluded order-preserving linear relations when p,q are non-zero.

Along the same lines, a natural and fairly accessible computational experiment would venture further outside of $\mathcal{D}_1$. It is motivated by the discovery (95). Any exhaustive study of the ensemble $\mathcal{D}$ is impractical until a reliable arbitrary-precision implementation of high-order derivatives for $\mathrm{Li}_s(x)$ with respect to s is completed. Hence, in light of (96), (97) and (98) it makes sense to hunt for all relations of weight at most 20 with total derivative weight 2, say.

As mentioned above, this study has underscored the need for high-precision evaluations of special functions in this research. This has spurred one of us (Crandall) to compile a set of unified and rapidly convergent algorithms (some new, some gleaned from existing literature) for a variety of special functions, suitable for practical implementation and efficient for very high-precision computation [22]. Some of these schemes were subsequently applied in this study. For instance, in regard to the above proposal to search for such as the $\zeta''(4)$ conjecture, the formula (54) [22, (51), p. 35] can be used to calculate d-th order derivatives $\mathrm{Li}_s^{(d)}(n)$ at arbitrary integers n.

But it is clear that substantial additional computational work is required. Since, as illustrated, the polylogarithms and their relatives are central to a great deal of mathematics and mathematical physics [4, 16, 28], such an effort is bound to pay off in the near future.

We conclude by re-emphasising the remarkable effectiveness of our computational strategy. The innocent looking sum $\mathcal{U}(50,50,0,0)$ mentioned inter alia can be generalized to an MTW sum having 100 arbitrary parameters:

$$\omega(s_1,\ldots,s_{50}\mid t_1,\ldots,t_{50}) := \sum_{\substack{m_1,\ldots,m_{50},n_1,\ldots,n_{50}>0\\ \sum_{i=1}^{50} m_i=\sum_{j=1}^{50} n_j}} \prod_{i=1}^{50}\frac{1}{{m_i}^{s_i}}\prod_{j=1}^{50}\frac{1}{{n_j}^{t_j}}. \tag{134}$$

We challenge readers to directly evaluate this sum.

8.1 Open theoretical questions

- Which $U_s(m, n)$ have closed forms?
- Find extensions of the exponential generating functions for $\mathcal{U}_s$ in Section 3.5 to more general s_j, t_k.
- Find extensions of the exponential generating functions for $\mathcal{U}_s$ in Section 3.5 to MTW's involving derivatives.
- **Conjecture**: all MTW relations and evaluations 'arise' from the results of Section 5 or from differentiating reflection formulas for MZV's.

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References

[1] T. Amdeberhan, M. Coffey, O. Espinosa, C. Koutschan, D. Manna, and V. Moll. Integrals of powers of loggamma. *Proc. Amer. Math. Soc.*, 139(2):535–545, 2010.

[2] G. E. Andrews, R. Askey, and R. Roy. *Special Functions.* Cambridge University Press, Cambridge, 1999.

[3] T. M. Apostol. Formulas for higher derivatives of the Riemann zeta function. *Mathematics of Computation*, 44:223–232, 1985.

[4] D. Bailey, R. Barrio, and J. Borwein. High-precision computation: Mathematical physics and dynamics. *Applied Mathematics and Computation*, In press 2012.

[5] D. Bailey, D. Borwein, and J. Borwein. On Eulerian log–Gamma integrals and Tornheim–Witten zeta functions. Preprint, February 2012.

[6] D. H. Bailey, J. M. Borwein, and R. E. Crandall. On the Khintchine constant. *Mathematics of Computation*, 66:417–431, 1997.

[7] D. H. Bailey and D. J. Broadhurst. Parallel integer relation detection: Techniques and applications. *Mathematics of Computation*, 70:1719–1736, 2000.

[8] D. H. Bailey, Y. Hida, X. S. Li, and B. Thompson. ARPREC: An arbitrary precision computation package. 2002.

[9] D. H. Bailey, X. S. Li, and K. Jeyabalan. A comparison of three high-precision quadrature schemes. *Experimental Mathematics*, 14:317–329, 2005.

[10] D. Borwein, J. Borwein, and R. Girgensohn. Explicit evaluation of Euler sums. *Proc. Edin. Math. Soc.*, 38:273–294, 1995.

[11] D. Borwein, J. M. Borwein, A. Straub, and J. Wan. Log-sine evaluations of Mahler measures, Part II. *Integers*, In press 2012.

[12] J. Borwein. Hilbert inequalities and Witten zeta-functions. *Proc. Amer. Math. Soc.*, 115(2):125–137, 2008.

[13] J. M. Borwein and D. H. Bailey. *Mathematics by Experiment.* A. K. Peters, 2nd edition, 2008.

[14] J. M. Borwein, D. M. Bradley, D. J. Broadhurst, and P. Lisoněk. Special values of multidimensional polylogarithms. *Trans. Amer. Math. Soc.*, 353(3):907–941, 2001.

[15] J. M. Borwein, D. M. Bradley, and R. E. Crandall. Computational strategies for the Riemann zeta function. *Journal of Computational and Applied Mathemataics*, 121:247–296, 2000.

[16] J. M. Borwein and A. Straub. Special values of generalized log-sine integrals. *Proceedings of ISSAC 2011 (International Symposium on Symbolic and Algebraic Computation)*, March 2011.

[17] J. M. Borwein and A. Straub. Log-sine evaluations of Mahler measures. *J. Aust Math. Soc.* Available at http://carma.newcastle.edu.au/jon/logsin.pdf, In press 2012.

[18] P. Borwein. An efficient algorithm for the Riemann zeta function. *Canadian Mathematical Society Conference Proceedings*, 27:29–34, 2000.

[19] D. M. Bradley and X. Zhou. On Mordell-Tornheim sums and multiple zeta values. *Ann. Sci. Math. Quebec*, 34:15–23, 2010.

[20] B. K. Choudhury. The Riemann zeta-function and its derivatives. *Proceedings of the Royal Society: Mathematical and Physical Sciences*, 450:477–499, 1995.

[21] H. Cohen, F. Villegas, and D. Zagier. Convergence acceleration of alternating series. *Experimental Math.*, 9:3–12, 2000.

[22] R. Crandall. Unified algorithms for polylogarithm, L-series, and zeta variants. 2012. Available at http://www.perfscipress.com/papers/UniversalTOC25.pdf.

[23] O. Espinosa and V. Moll. The evaluation of Tornheim double sums. Part I. *Journal of Number Theory*, 116:200–229, 2006.

[24] O. Espinosa and V. Moll. The evaluation of Tornheim double sums. Part II. *Journal of Number Theory*, 22:55–99, 2010.

[25] M. Kalmykov. About higher order ϵ-expansion of some massive two- and three-loop master-integrals. *Nuclear Physics B*, 718:276–292, July 2005.

[26] Y. Komori. An integral representation of the Mordell-Tornheim double zeta function and its values at non-positive integers. *Ramanujan J.*, 17(2):163–183, 2008.

[27] L. Lewin. On the evaluation of log-sine integrals. *The Mathematical Gazette*, 42:125–128, 1958.

[28] L. Lewin. *Polylogarithms and associated functions*. North Holland, 1981.

[29] K. Matsumoto. On Mordell-Tornheim and other multiple zeta-functions. *Proceedings of the Session in Analytic Number Theory and Diophantine Equations*, Bonner Math. Schriften, vol. 360, University of Bonn, 2003.

[30] N. Nielsen. *Handbuch der theorie der Gammafunction*. Druck und Verlag von B.G. Teubner, Leipzig, 1906.

[31] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark. *NIST Handbook of Mathematical Functions*. Cambridge University Press, 2010.

[32] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark. NIST Digital Handbook of Mathematical Functions. 2012.

[33] K. Onodera. Analytic properties of multiple zeta-functions in several variables. *Number theory. Dev. Math.*, 15:153–173, 2006.

[34] K. Onodera. Generalized log sine integrals and the Mordell-Tornheim zeta values. *Trans. Amer. Math. Soc.*, 363(3):1463–1485, 2011.

[35] L. Tornheim. Harmonic double series. *Amer. J. Math.*, 72:303–324, 1950.

[36] H. Tsumura. Combinatorial relations for Euler-Zagier sums. *Acta Arith.*, 111(1):27–42, 2004.

[37] H. Tsumura. On Mordell-Tornheim zeta values. *Proc. Amer. Math. Soc.*, 133:2387–2393, 2005.