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COMPUTATION AND THEORY OF EXTENDED MORDELL-TORNHEIM-WITTEN SUMS

DAVID H. BAILEY, JONATHAN M. BORWEIN, AND RICHARD E. CRANDALL

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 this, we make use of symbolic integration, high precision numerical integration, and some interesting combinatorics and special-function theory. Our original motivation was to represent unresolved constructs such as Eulerian log-gamma integrals. We are able to resolve all such integrals in terms of an MTW basis. We also present, for a substantial subset of MTW values, 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.

1. Introduction

We define an ensemble of extended Mordell–Tornheim–Witten (MTW) zeta function values [4, 11, 17, 21, 22, 33–35]. There is by now a huge body of 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 unresolved constructs such as Eulerian log-gamma integrals. 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

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

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 paper is as follows. In Section 2 we introduce an ensemble $\mathcal{D}$ capturing the values we wish to study and we provide some effective integral

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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 first provide a 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.

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 $\mathcal{L}G_n$ 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* [12] 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.

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 [27], 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 [4] introduced and discussed an apparently-novel generalized MTW zeta function for positive integers M, N and nonnegative integers s_i, t_j—with constraints $M \geq N \geq 1$—together with a polylogarithm-integral representation:

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

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

Here the *polylogarithm of order* s denotes $\mathrm{Li}_s(z) := \sum_{n\geq 1} z^n/n^s$ and its analytic extensions [26] and the (complex) number s is its *order*.

Note that if parameters are zero, there are convergence issues with this integral representation. One may use principal-value calculus, or an alternative representation such as (11) below. When $N = 1$ the representation (3) devolves to the classic MTW form, in that

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

We need a wider *MTW ensemble* involving outer derivatives, according to

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

$$(5)\qquad = \frac{1}{2\pi}\int_0^{2\pi} \prod_{j=1}^M \mathrm{Li}_{s_j}^{(d_j)}\left(e^{i\theta}\right) \prod_{k=1}^N \mathrm{Li}_{t_k}^{(e_k)}\left(e^{-i\theta}\right)\,\mathrm{d}\theta,$$

where the s-th outer derivative of a polylogarithm is denoted $\mathrm{Li}_s^{(d)}(z) := \left(\frac{\partial}{\partial s}\right)^d \mathrm{Li}_s(z)$. We emphasize that all ω are real since we integrate over a full period or more directly since the summand is real. Consistent with earlier usage, we now refer to $M+N$ as the *depth* and $\sum_{j=1}^M(s_j+d_j)+\sum_{k=1}^N(t_k+e_k)$ as the *weight* of ω.

To summarize, we consider an MTW ensemble comprising the set

(6)

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

2.1. **Important subensembles.** We shall, in our resolution of log-gamma integrals especially, engage MTW constructs using only parameters 1 or 0. We define $\mathcal{U}(m,n,p,q)$ to vanish if $mn=0$; otherwise if $m\ge n$ we define

$$\mathcal{U}(m,n,p,q) := \frac{1}{2\pi}\int_0^{2\pi} \mathrm{Li}_1\left(e^{i\theta}\right)^{m-p}\mathrm{Li}_1^{(1)}\left(e^{i\theta}\right)^{p}\mathrm{Li}_1\left(e^{-i\theta}\right)^{n-q}\mathrm{Li}_1^{(1)}\left(e^{-i\theta}\right)^{q}\,\mathrm{d}\theta$$

$$(7)\qquad = \omega\left(\begin{array}{c|c} \mathbf{1}_m & \mathbf{1}_n \\ \mathbf{1}_p\mathbf{0}_{m-p} & \mathbf{1}_q\mathbf{0}_{n-q} \end{array}\right),$$

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

$$\mathcal{D}_1 := \{\mathcal{U}(m,n,p,q):\ p\le m\ge n\ge q\}.$$

Another subensemble $\mathcal{D}_0\subset\mathcal{D}_1\subset\mathcal{D}$ is a *derivative-free* set of MTWs of the form $\mathcal{D}_0 := \{\mathcal{U}(M,N,0,0) : M\ge N\ge 1\}$, 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

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

in which an element of $\mathcal{D}_0(s)$ has the form $\omega(\mathbf{s}_M \mid \mathbf{s}_N)$, for $s=1,2,\ldots$, and $\mathcal{D}_0(1)=\mathcal{D}_0$. For economy of notation, we shall sometimes write $\mathcal{U}_s(M,N) := \mathcal{U}_s(M,N,0,0)$.

2.2. **Closed forms for certain MTWs.** For $N=1$ in definition (2) we have:

$$(8)\qquad \omega(r\mid s) = \zeta(r+s),$$

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

$$(10)\qquad \omega(r,0\mid s) = \omega(0,r\mid s) = \zeta(s,r),$$

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 [13] and are believed to be *irreducible*; see also [9,34,35]. Such beginning evaluations use simple combinatorics;

later in Section 5 we shall see much more sophisticated combinatorics come into play.

This is the classic MTW (1), with a useful pure-real integral alternative to (3). The incomplete gamma function integral [20], lets one write

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

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

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

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 $t > 4$. Multidimensional analytic continuation is patently nontrivial. Indeed, the 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 we might infer $\omega(0,0,0,0 \mid 0) = \zeta(0)^4 \stackrel{?}{=} \frac{1}{16}$. This shows hat analytic continuation of MTWs (even MZVs) must be performed carefully [24, 27, 31]. Via these definite-integration techniques or sheer combinatorics, for t in its region of absolute convergence, we have the 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* [30] as discussed prior to (71).

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

Whereas our previous section exhibits closed forms for $N = 1$ (i.e., classic MTW forms of type (4)), we now address the important class of resolvable MTWs for general $N > 1$.

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 $a > 0$ [30, Equation (5.12.5)] records the beta function evaluation:

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

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:

$$\begin{aligned} &9600\,\pi^2\zeta\left(5\right)\zeta\left(3\right) + 600\,\zeta^2\left(3\right)\pi^4 + \frac{77587}{8316}\,\pi^{10} \\ &\qquad + 144000\,\zeta\left(7\right)\zeta\left(3\right) + 72000\,\zeta^2\left(5\right). \end{aligned} \tag{18}$$

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

$$\begin{aligned} &8.810791818778736904649020672776766667353256223589929081929162096 3\\ &955610495437473402013805397251288 49 \times 10^{31}. \end{aligned} \tag{19}$$

This was in full agreement with our numerical integration scheme of the next section. ♢

The *log-sine-cosine integrals* given by

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

have been considered by Lewin, [25,26] and in physical applications; see for instance [23]. From the form given in [10], Lewin's result can be restated as

(21)

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

This is closely linked to (14); see also [32]. 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 address the generating function $\mathcal{V}(x,y)$, we recall expansions of the Gamma function itself. In [25, 30] is the classical formula

$$\log \Gamma(1-z) \;=\; \gamma z \;+\; \sum_{n>1} \zeta(n)\frac{z^n}{n} \text{ or } e^{-\gamma z}\Gamma(1-z) \;=\; \exp\left\{\sum_{n>1} \frac{\zeta(n) z^n}{n}\right\}, \tag{23}$$

everything being convergent for $|z| < 1$. This leads immediately to a powerful exponential series representation for our generating function

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

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

Theorem 2 (Evaluation of $\mathcal{U}(M,N)$)**.** *For any integers $M \ge N \ge 1$ we have that $\mathcal{U}(M,N) = \omega(\mathbf{1}_M \mid \mathbf{1}_N) \in \mathcal{D}_0$ lies in the ring $\mathcal{R} := \langle \mathcal{Q} \cup \{\pi\} \cup \{\zeta(3), \zeta(5), \zeta(7), \dots\}\rangle$. In particular, for $M \ge N$, and setting $\mathcal{U}(M,0) := 1$, the general expression is:*

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

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 $\exp\{Q\} = 1+Q+Q^2/2!+\dots$ gives a finite form for a coefficient $\mathcal{U}(M,N)$. ☐

A second proof again connects the present theory with log-sine integrals:

Proof (Alternative proof of Theorem 2). From the logarithmic form of Li_1 (54), we have

(25)

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

[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.

Now, upon expanding the integrand we can cast this $\mathcal{U}$ as a finite superposition of log-sine integrals. Specifically, from [15] 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 [15] provide a full generating function:

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

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 $\mathcal{U}$ functions.** Remarkably, extreme-precision numerical experiments, as detailed later, discovered a unique sum rule amongst $\mathcal{U}$ functions with a fixed *even* order $M+N$. Eventually, we were led 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 (59)), 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* (104). 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 form

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

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 [26, §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 nonnegative 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 previously, 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

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

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 [15], [25, §7.9.5] and [29, §5.15]. More details can be found in [9, pp. 281–282] and [25, §7.9.2]. ☐

Remark 1. We note that [25, (7.128)] gives $I(2,1,2) = 8\,\zeta\,(5) - \frac{2}{3}\,\zeta\,(3)\,\pi^2$ and an incorrect value for $I(3,1,2) = 6\,\zeta^2\,(3) - \frac{1}{105}\,\pi^6$. ♢

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 §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

$$\mathcal{U}_s(m,n) := \frac{1}{2\pi} \int_0^{2\pi} \mathrm{Li}_s\left(e^{i\theta}\right)^m \mathrm{Li}_s\left(e^{-i\theta}\right)^n \, d\theta \;=\; \omega\begin{pmatrix} \mathbf{s}_m & \mid & \mathbf{s}_n & 0 \\ \mathbf{0}_m & \mid & \mathbf{0}_n & \end{pmatrix}. \tag{31}$$

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 $\mathcal{U}_s(1,1) = \zeta(2s)$. Likewise, $\mathcal{U}_s(2,1) = \omega(s,s,s)$, which is evaluable by Theorem 7 and for which classical closed forms are recorded in [21, Eqns. (1.20) and (1.21)]. Likewise, $\mathcal{U}_s(n,1)$ is evaluable for positive integer n.

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

$$\mathcal{V}_2(x,y) := \sum_{m,n \geq 0} \mathcal{U}_2(m,n) \frac{x^m\, y^n}{m!\, n!}. \tag{32}$$

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

$$\mathcal{V}_2(ix, iy) := \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{(y-x))\mathrm{Cl}_2(\theta)} \cos\left(\frac{\left(2\,\pi^2+3\,\theta^2-6\,\pi\,\theta\right)}{12}\,(y+x)\right)\mathrm{d}\theta + i\,\frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{(y-x))\mathrm{Cl}_2(\theta)} \sin\left(\frac{\left(2\,\pi^2+3\,\theta^2-6\,\pi\,\theta\right)}{12}\,(y+x)\right)\mathrm{d}\theta, \tag{33}$$

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 [26, 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 [30, §7.2(iii)], to be

$$2\pi\,\mathcal{V}_2(ix, ix) = 2\sqrt{\frac{\pi}{x}}\left(\cos\left(\frac{x\pi^2}{6}\right)C\left(\sqrt{\pi x}\right)+\sin\left(\frac{x\pi^2}{6}\right)S\left(\sqrt{\pi x}\right)\right) + i\,2\sqrt{\frac{\pi}{x}}\left(\cos\left(\frac{x\pi^2}{6}\right)S\left(\sqrt{\pi x}\right)-\sin\left(\frac{x\pi^2}{6}\right)C\left(\sqrt{\pi x}\right)\right). \tag{34}$$

On using the series representations [30, Eqns. (7.6.4) & (7.6.6)] we arrive at:

$$\mathrm{Re}\ \mathcal{V}_2(ix, ix) = \cos\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^\infty \frac{(-1)^n\,\pi^{4\,n}}{2^{2\,n+2}\,(2\,n)!\,(4\,n+1)}\,x^{2\,n} + \sin\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^\infty \frac{(-1)^n\,\pi^{4\,n+2}}{2^{2\,n+3}\,(2\,n+1)!\,(4\,n+3)}\,x^{2\,n+1}, \tag{35}$$

$$\mathrm{Im}\ \mathcal{V}_2(ix, ix) = -\sin\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^\infty \frac{(-1)^n\,\pi^{4\,n}}{2^{2\,n+2}\,(2\,n)!\,(4\,n+1)}\,x^{2\,n} + \cos\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^\infty \frac{(-1)^n\,\pi^{4\,n+2}}{2^{2\,n+3}\,(2\,n+1)!\,(4\,n+3)}\,x^{2\,n+1}. \tag{36}$$

We note that $\mathrm{Re}\mathcal{V}_2(ix, ix)$ is an even function and $\mathrm{Im}\mathcal{V}_2(ix, ix)$ is odd. Then, on comparing (32) with $ix = iy$ to (35) or (36) we arrive at:

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

$$\sum_{m=1}^{2p-1}\binom{2p}{m}\mathcal{U}_2(m, 2p-m) = (-1)^p\,q_{2p}\,\pi^{4p}, \tag{37}$$

$$\sum_{m=1}^{2p}\binom{2p+1}{m}\mathcal{U}_2(m, 2p+1-m) = (-1)^p\,q_{2p+1}\,\pi^{4p+2}. \tag{38}$$

3.5.1. *The $\mathcal{U}_s$ sums when $s \geq 3$.* It is possible to undertake the same analysis generally.

Example 4. From the evaluation Gl_3 [26, Eqn. (22), p. 297] may deduce that

$$\mathcal{V}_3(x, -x) = \frac{1}{\pi}\int_0^\pi \cos\left(\left(\pi^2-\theta^2\right)\frac{\theta}{6}\,x\right)\mathrm{d}\theta. \tag{39}$$

The Taylor series commences

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

Then $6\mathcal{U}_3(2,1)$ is the next coefficient and all terms have the weight one would predict. $\diamondsuit$

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

$$\mathrm{Gl}_n\left(\theta\right) = (-1)^{1+\lfloor n/2\rfloor} 2^{n-1} \frac{\pi^n}{n!} B_n\left(\frac{\theta}{2\pi}\right) \tag{40}$$

for $n > 1$ where B_n is the n-th *Bernoulli polynomial* [26, Eqn. (22), p. 300] and $0 \le \theta \le 2\pi$. 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

$$\mathcal{V}_{2n+1}(x,-x) = \frac{1}{2\pi}\int_0^{2\pi} \cos\left(\mathrm{Gl}_{2n+1}\left(\theta\right) x\right)\,\mathrm{d}\theta, \tag{41}$$

$$\mathcal{V}_{2n}(ix,ix) = \frac{1}{2\pi}\int_0^{2\pi} \exp\left(i\mathrm{Gl}_{2n}\left(\theta\right) x\right)\,\mathrm{d}\theta. \tag{42}$$

In each case substitution of (40) and term-by-term expansion of cos or sin leads to an expression for the coefficients; note that $\mathrm{Gl}_n\left(\theta\right)$ is an homogeneous two-variable polynomial in π and θ with each monomial of degree n. Indeed, we are thus led to explicit formulas

$$r_m(s) := (-1)^m \frac{4^{m-1}}{(2m)!\,\pi}\int_0^{2\pi}\left(\frac{(-1)^{1+\lfloor s/2\rfloor}}{s!}\left(2\pi\right)^s B_n\left(\frac{\theta}{2\pi}\right)\right)^{2\,m}\,\mathrm{d}\theta \tag{43}$$

$$i_m(s) := (-1)^m \frac{2\,4^{m-1}}{(2m+1)!\,\pi}\int_0^{2\pi}\left(\frac{(-1)^{1+\lfloor s/2\rfloor}}{s!}\left(2\pi\right)^s B_n\left(\frac{\theta}{2\pi}\right)\right)^{2\,m+1}\,\mathrm{d}\theta \tag{44}$$

for the real and imaginary coefficients of order $2m$. (These expand as finite sums, but may painlessly be integrated symbolically.) The imaginary part 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.*

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 [4] gives formulas such as: when $s = n$ is a positive integer,

$$\mathrm{Li}_n(z) = {\sum_{m=0}^{\infty}}' \zeta(n-m)\frac{\log^m z}{m!} + \frac{\log^{n-1} z}{(n-1)!}\left(H_{n-1} - \log(-\log z)\right), \tag{45}$$

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,

$$\mathrm{Li}_s(z) = \sum_{m\geq 0} \zeta(s-m)\frac{\log^m z}{m!} + \Gamma(1-s)(-\log z)^{s-1}. \tag{46}$$

Note in formula (45), 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

$$\mathrm{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s}. \tag{47}$$

In fact, we found that formula (47) is generally faster than (45) whenever $|z| < 1/4$, at least for precision levels in the range of 100 to 4000 digits.

4.1.1. *Derivatives of general order polylogarithms.* For integer $k > 0$ we have [20, §9, Eqn. (51)]: for $|\log z| < 2\pi$ and $\tau \in [0, 1)$:

$$\mathrm{Li}_{k+1+\tau}(z) = \sum_{0\leq n\neq k} \zeta(k+1+\tau-n)\frac{\log^n z}{n!} + \frac{\log^k}{k!}\sum_{j=0}^{\infty} c_{k,j}(\mathcal{L})\,\tau^j, \tag{48}$$

where $\mathcal{L} := \log(-\log z)$ and the c coefficients engage the Stieltjes constants [20, §7.1]:

$$c_{k,j}(\mathcal{L}) = \frac{(-1)^j}{j!}\gamma_j - b_{k,j+1}(\mathcal{L}). \tag{49}$$

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

$$b_{k,j}(\mathcal{L}) := \sum_{\substack{p+t+q=j\\ p,t,q\geq 0}} \frac{\mathcal{L}^{\,p}}{p!}\frac{\Gamma^{(t)}(1)}{t!}(-1)^{t+q} f_k(q), \tag{50}$$

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

$$f_{k,q} = \sum_{h=0}^{q} \frac{(-1)^h}{k^h} f_{k-1,q-h}. \tag{51}$$

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 (48).

To obtain first (or higher) derivatives $\mathrm{Li}_{k+1}^{(1)}(z)$, we differentiate (48) at zero and so require the evaluation $c_{k,1}$. With $k = 0$ and $j = 1$, this supplies (53) below.

4.1.2. *The special case $s = 1$ and $z = e^{i\theta}$.* Most importantly, we may write, for $0 < \theta < 2\pi$,

$$\mathrm{Li}_1(e^{i\theta}) = -\log\left(2\sin\left(\frac{\theta}{2}\right)\right) + \frac{(\pi-\theta)}{2}i. \tag{52}$$

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

$$L'_1(z) = \sum_{n=1}^{\infty} \zeta'\left(1-n\right) \frac{\log^n z}{n!} - \gamma_1 - \frac{1}{12}\,\pi^2 - \frac{1}{2}\,\left(\gamma + \log\left(-\log z\right)\right)^2, \tag{53}$$

which, as before, is valid whenever $|\log z| < 2\pi$. Here γ_1 is the *second Stieltjes constant* [2, 20]. For small $|z|$, it again suffices to use the elementary form

$$\mathrm{Li}'_s(z) = -\sum_{n=1}^{\infty} \frac{z^k \log k}{k^s}. \tag{54}$$

Relation (53) can be applied to yield the formula

$$\mathrm{Li}'_1(e^{i\theta}) = \sum_{n=1}^{\infty} \zeta'\left(1-n\right) \frac{(i\theta)^n}{n!} - \gamma_1 - \frac{1}{12}\,\pi^2 - \frac{1}{2}\,\left(\gamma + \log\left(-i\theta\right)\right)^2, \tag{55}$$

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 [20].

4.2. **ζ at integer arguments.** Using formulas (45) and (46) requires precomputed values of the zeta function and its derivatives at integer arguments; see [2, 18]. One fairly efficient algorithm for computing $\zeta(n)$ for integer $n > 1$ is the following, given by Peter Borwein [16]: Choose $N > 1.2\cdot D$, where D is the number of correct digits required. Then

$$\zeta(s) \approx -2^{-N}(1-2^{1-s})^{-1} \sum_{i=0}^{2N-1} \frac{(-1)^i \sum_{j=-1}^{i-1} u_j}{(i+1)^s}, \tag{56}$$

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 even integer arguments.* As we require $\zeta(n)$ for many integers, the following approach, used in [5], is more efficient. First, to compute $\zeta(2n)$, observe that

$$\begin{aligned} \coth(\pi x) &= \frac{-2}{\pi x}\sum_{k=0}^{\infty} \zeta(2k)(-1)^k x^{2k} \;=\; \cosh(\pi x)/\sinh(\pi x) \\ &= \frac{1}{\pi x}\cdot\frac{1+(\pi x)^2/2!+(\pi x)^4/4!+(\pi x)^6/6!+\cdots}{1+(\pi x)^2/3!+(\pi x)^4/5!+(\pi x)^6/7!+\cdots}. \end{aligned} \tag{57}$$

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

$$R_{k+1}(x) := R_k(x) + [1 - Q(x)\cdot R_k(x)]\cdot R_k(x), \tag{58}$$

where 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 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 [5]. Note that $\zeta(0) = -1/2$.

4.2.2. *ζ at positive odd integer arguments.* The *Bernoulli numbers* B_{2k} are also needed. They can now be obtained from [30, Eqn. (25.6.2)]

$$B_{2k} = (-1)^{k+1}\frac{2(2k)!\zeta(2k)}{(2\pi)^{2k}}. \tag{59}$$

The positive odd-indexed zeta values can be efficiently computed using these two Ramanujan-style formulas [5, 14]:

$$\begin{aligned} \zeta(4N+3) &= -2\sum_{k=1}^{\infty}\frac{1}{k^{4N+3}(\exp(2k\pi)-1)} \\ &\quad -\pi(2\pi)^{4N+2}\sum_{k=0}^{2N+2}(-1)^k\frac{B_{2k}B_{4N+4-2k}}{(2k)!(4N+4-2k)!}, \\ \zeta(4N+1) &= -\frac{1}{N}\sum_{k=1}^{\infty}\frac{(2\pi k+2N)\exp(2\pi k)-2N}{k^{4N+1}(\exp(2k\pi)-1)^2} \\ &\quad -\frac{1}{2N}\pi(2\pi)^{4N}\sum_{k=1}^{2N+1}(-1)^k\frac{B_{2k}B_{4N+2-2k}}{(2k-1)!(4N+2-2k)!}. \end{aligned} \tag{60}$$

4.2.3. *ζ at negative integer arguments.* Finally, the zeta function can be evaluated at negative integers by the following well-known formulas [30, (25.6.3), (25.6.4)]:

$$\zeta(-2n+1) = -\frac{B_{2n}}{2n} \qquad \text{and} \qquad \zeta(-2n) = 0. \tag{61}$$

4.3. **ζ' at integer arguments.** Precomputed values of the zeta derivative function are prerequisite for the efficient use of formulas (53) and (55).

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. The scheme is illustrated in the following *Mathematica* code (for argument `ss` and precision `prec` digits) (see [20] and more general acceleration methods in [19]):

```
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.* The functional equation

$$\zeta(s) = 2(2\pi)^{s-1} \sin \frac{\pi s}{2} \Gamma(1-s)\, \zeta(1-s)$$

lets one extract $\zeta'(0) = -\frac{1}{2}\log 2\pi$ and for even $m = 2, 4, 6, \ldots$

$$\zeta'(-m) := \frac{d}{ds}\zeta(s)|_{s=-m} = \frac{(-1)^{m/2} m!}{2^{m+1}\pi^m}\, \zeta(m+1) \tag{62}$$

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

$$\zeta'(-m) = \zeta(-m)\left(\gamma + \log 2\pi - H_m - \frac{\zeta'(m+1)}{\zeta(m+1)}\right). \tag{63}$$

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 [30, (5.7.1) and (5.7.2)] that

$$\Gamma(z+1)\, \mathcal{C}(z) = z\, \Gamma(z)\, \mathcal{C}(z) = z, \tag{64}$$

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

$$(k-1)c_k = \gamma c_{k-1} - \zeta(2)\, c_{k-2} + \zeta(3)\, c_{k-3} - \cdots + (-1)^k\, \zeta(k-1)\, c_1 \tag{65}$$

Thus, differentiating (64) by Leibniz' formula, for $n \geq 1$ we have

$$g_n = -\sum_{k=0}^{n-1} \frac{n!}{k!}\, g_k\, c_{n+1-k}. \tag{66}$$

More generally, for positive integer m we have

$$\Gamma(z+m)\; \mathcal{C}(z) = (z)_m, \tag{67}$$

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 (67) and obtain

$$g_n(m) = -\sum_{k=0}^{n-1} \frac{n!}{k!}\, g_k(m)\, c_{n+1-k} + \frac{D_m^{n+1}}{n+1}. \tag{68}$$

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

$$D_m^n = \sum_{k=0}^{m-n} s\,(m, k+n)\,(k+1)_n\,(m-1)^k = (n+1)!\,(-1)^{m+n+1} s\,(m, 1+n)\,. \tag{69}$$

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

$$\frac{g_n(m)}{n!} = -\sum_{k=0}^{n-1} \frac{g_k(m)}{k!}\, c_{n+1-k} + |s(m, 1+n)|, \tag{70}$$

where for integer $n, k \geq 0$,

$$s(n,k) = s(n-1, k-1) - (n-1)\, s(n-1, k)\,; \tag{71}$$

see [30, 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 $\kappa := -\log(2\pi) - \frac{1}{2}\pi i$, we have Apostol's explicit formulas [30, (25.6.13) and (25.6.14)]:

$$(-1)^k \zeta^{(k)}(1-2n) = \frac{2(-1)^n}{(2\pi)^{2n}} \sum_{m=0}^{k} \sum_{r=0}^{m} \binom{k}{m} \binom{m}{r} \mathrm{Re}(\kappa^{k-m})\, \Gamma^{(r)}(2n)\, \zeta^{(m-r)}(2n)\,, \tag{72}$$

$$\begin{aligned} &(-1)^k \zeta^{(k)}(-2n) \\ &\quad = \frac{2(-1)^n}{(2\pi)^{2n+1}} \sum_{m=0}^{k} \sum_{r=0}^{m} \binom{k}{m} \binom{m}{r} \mathrm{Im}(\kappa^{k-m})\, \Gamma^{(r)}(2n+1)\, \zeta^{(m-r)}(2n+1)\,. \end{aligned} \tag{73}$$

Since in (68) only the initial conditions rely on m, equations (72) and (73) are well fitted to work with (68) (along with (71), and (65)).

4.5. **Tanh-sinh quadrature.** We address efficient performance of quadrature as needed, e.g., for the $\mathcal{U}$ constants (7). Since integrands in (7) are typically rather badly behaved, we recommend *tanh-sinh quadrature*, which is remarkably insensitive to singularities at endpoints of the interval of integration. We approximate the integral of $f(x)$ on $(-1, 1)$ as

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\,\mathrm{d}t \;\approx\; h \sum_{j=-N}^{N} w_j f(x_j), \tag{74}$$

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

$$\begin{aligned} x_j &= g(hj) = \tanh\left(\pi/2 \cdot \sinh(hj)\right), \\ w_j &= g'(hj) = \pi/2 \cdot \cosh(hj)/\cosh\left(\pi/2 \cdot \sinh(hj)\right)^2, \end{aligned} \tag{75}$$

where N is chosen so terms of the summation beyond N are smaller in absolute value than the "epsilon" of the numeric precision being used. The abscissas x_j and weights w_j can be precomputed, and then applied to all quadrature calculations. For many integrand functions, including those in (7), reducing h by half in (74) and (75) roughly doubles the number of correct digits, provided calculations are done to a precision level at least that desired for the final result. Full details are given in [8].

For our $\mathcal{U}$ calculations, it suffices to integrate from 0 to π, divided by π, provided we integrate the real part of the integrand. Also, when computing $\mathcal{U}(m, n, p, q)$ for many values of m, n, p and q, it is much faster to precompute the polylog functions and derivative functions (sans the exponents) at each of the tanh-sinh abscissa points x_j. Thence, during a quadrature, an evaluation in (7) merely consists of table look-ups and a few multiplications for each function evaluation. In our implementations, quadrature calculations were thus accelerated by a factor of over 1000.

5. More recondite MTW interrelations

We now return to our subjects 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 [4]). *Let nonnegative integers a, b, c and r, s, t be given. Set $N := r + s + t$. Define the shorthand notation*

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

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

$$\delta(r, s, t) = \sum_{i=1}^{r} \binom{r+s-i-1}{s-1} \delta\,(i, 0, N-i) + \sum_{i=1}^{s} \binom{r+s-i-1}{r-1} \delta\,(0, i, N-i)\,. \tag{76}$$

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

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

$$d(r, s, t-1) = d(r-1, s, t) + d(r, s-1, t) \tag{77}$$

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 (77) 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 (77) 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 (76) 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 nonnegative integers q, r, s, t, assume that $d\,(q, r, s, t)$ satisfies the recurrence*

$$d\,(q, r, s, t) = d\,(q-1, r, s, t+1) + d\,(q, r-1, s, t+1) + d\,(r, s-1, t+1)\,. \tag{78}$$

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 5 (Values of δ)**.** Again we use the shorthand notation

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

The techniques in [20] 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

$$\omega_{1,0,1}(1,0,3) = 0.14042163138773371925054281123123563768136197000104827665935...$$
$$\omega_{1,0,1}(2,0,2) = 0.40696928390140268694035563517591371639834128770661373815447...$$
$$\omega_{1,0,1}(1,1,2) = 0.43097253394888316942248176511038963971077201581912157 52309...$$

and

$$\omega_{0,1,1}(2,1,1) = 3.00297121355668005079211509351534225995879828374320045 9879...$$

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

$$\begin{aligned} &= 0.140421631387733719247 + 0.290550902561149450 12 - 0.430972533948883169 42 \\ &= 0.00000000000000000000..., \end{aligned}$$

both in accord with Theorem 7. Also, PSLQ run on the above data predicts that

$$\zeta''(4) \overset{?}{=} 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2) - 2\,\omega_{1,0,1}(2,0,2), \tag{79}$$

whose discovery also validates the effectiveness of our high-precision techniques. $\diamondsuit$

From (79) we see less trivial derivative relations lie within $\mathcal{D}$ than within $\mathcal{D}_1$. As noted,

$$\mathcal{U}(1,1,1,1) = \omega\left(\begin{array}{c|c} 1 & 1 \\ 1 & 1 \end{array}\right) = \zeta''(2). \tag{80}$$

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

$$\omega\left(\begin{array}{cc|c} s, & 0 & t \\ a, & 0 & b \end{array}\right) = \zeta_{a,b}(t,s), \tag{81}$$

$$\omega\left(\begin{array}{cc|c} s, & t & 0 \\ a, & b & 0 \end{array}\right) = \zeta^{(a)}(s)\,\zeta^{(b)}(t). \tag{82}$$

We may now prove (79):

Proposition 1.

$$\zeta''(4) = 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2) - 2\,\omega_{1,0,1}(2,0,2). \tag{83}$$

Proof. First note that by (82),

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

Next the MZV reflection formula $\zeta(s,t) + \zeta(t,s) = \zeta(s)\zeta(t) - \zeta(s+t)$, (see [9]), 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 (81). Since $\omega_{1,1,0}(2,0,2) = 2\omega_{1,0,1}(2,1,1)$ by Theorem 7, our desired formula (83) is

$$\zeta''(4) + 2\,\omega_{1,0,1}(2,0,2) = 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2), \tag{84}$$

which is equivalent to

$$\zeta'(2)^2 = \omega_{1,1,0}(2,2,0) = 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2). \tag{85}$$

The final equality is another easy case of Theorem 7. □

5.2. **Relations when $M \geq N \geq 2$.** Since $\sum t_k = \sum s_j$, we deduce from (2), by a partial fraction argument that

Theorem 9 (Relations for general ω)**.**

$$\begin{aligned} &\sum_{k=1}^{N} \omega\left(\begin{array}{c|c} s_1, \ldots, s_M & t_1, \ldots, t_{k-1}, t_k - 1, t_{k+1}, \ldots, t_N \\ d_1, \ldots, d_M & e_1, \ldots e_N \end{array} \right) \\ &= \sum_{j=1}^{M} \omega\left(\begin{array}{c|c} s_1, \ldots, s_{j-1}, s_j - 1, s_{j+1}, \ldots, s_M & t_1, \ldots, t_N \\ d_1, \ldots, d_M & e_1, \ldots e_N \end{array} \right). \end{aligned} \tag{86}$$

When $N = 1$ and $M = 2$ this is precisely (77). For $N = 1$ and general M there is a result like Theorem 8. For $N > 1$ we find 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 arrive at:

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

$$\kappa(a_1, \ldots, a_n \mid b_1, \ldots, b_n) := \sum_{n_i > 0} \frac{1}{\prod_{i=1}^n {n_i}^{a_i} \prod_{j=1}^n {N_j}^{b_j}}, \tag{87}$$

for positive integers a_i and nonnegative b_j (with b_n large enough to assure convergence). Thence $\kappa(a_1, \ldots, a_n \mid b_1) = \omega(a_1, \ldots, a_n \mid b_1)$. Noting that κ is symmetric in the a_i we denote $\overrightarrow{a}$ to be the nonincreasing rearrangement of $\overline{a} := (a_1, a_2, \ldots, a_n)$. Let k be the largest index of a nonzero element in $\overrightarrow{a}$. The partial fraction above gives

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

We repeat this step until there are only $k-1$ nonzero 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 $\kappa(\overrightarrow{0} \mid \overline{b}) = \zeta(b_n, b_{n-1}, \ldots, b_1)$. 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 [34]. □

Tsimura [35] 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 [34]. As we discovered later, Theorem 10 was recently proven very neatly by explicit combinatorial methods in [17], which do not lend themselves to our algorithmic needs.

5.4. **Degenerate MTW derivatives with zero numerator values.** In Theorem 10 we include no derivative values—a zero value may still have a log term in the corresponding variable—nor about $N \geq 2$. For example, it appears unlikely that

$$\omega\left(\begin{array}{cc|c} 1\,, & 0 & 2 \\ 0\,, & 1 & 0 \end{array}\right) = \sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^{n-1} \frac{\log(n-m)}{m} \tag{88}$$

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

$$\omega\left(\begin{array}{cc|c} 0\,, & 0 & s \\ 0\,, & 1 & 0 \end{array}\right) = -\sum_{n=2}^{\infty} \frac{\log\Gamma(n)}{n^s}. \tag{89}$$

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:

$$\omega\left(\begin{array}{cc|c} q\,, & r & s \\ 0\,, & 1 & 0 \end{array}\right) = \frac{1}{\Gamma(s)} \int_0^{\infty} x^{s-1} \mathrm{Li}_q(e^{-x})\, \mathrm{Li}_r^{(1)}(e^{-x})\, \mathrm{d}x. \tag{90}$$

Though unlikely that MTW derivatives are finite superpositions of MZV derivatives, it is possible to go some distance in establishing (nonfinitary) relations. Consider the development

$$\begin{aligned}\omega\left(\begin{array}{cc|c} r\,, & 0 & s \\ 0\,, & 1 & 0 \end{array}\right) &= -\sum_{m,n\geq 1}\frac{1}{m^r}\log n\frac{1}{(m+n)^s} \\ &= -\sum_{N\geq 1}\frac{1}{N^s}\sum_{M=1}^{N-1}\frac{\log(N-M)}{M^r} \\ &= \zeta^{(1,0)}(s,r) + \sum_{k\geq 1}\frac{1}{k}\zeta(s+k,r-k).\end{aligned} \tag{91}$$

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

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 [4]—in that our log-gamma integrals $\mathcal{LG}_n$ lie in a specific algebra.

6.1. **Log-gamma representation.** We start, as in [4] with the Kummer series; see [1, p. 28], or [28, (15) p. 201]:

$$\begin{aligned}\log\Gamma(x) - \frac{1}{2}\log(2\pi) = &-\frac{1}{2}\log\left(2\sin(\pi x)\right) + \frac{1}{2}(1-2x)\left(\gamma+\log(2\pi)\right) \\ &+\frac{1}{\pi}\sum_{k=2}^{\infty}\frac{\log k}{k}\sin(2\pi k x)\end{aligned} \tag{92}$$

for $0 < x < 1$. With a view toward polylogarithm use, this can be written as

$$\log\Gamma\left(\frac{z}{2\pi}\right) - \frac{1}{2}\log 2\pi \;=\; A\,\mathrm{Li}_1(e^{iz}) + B\,\mathrm{Li}_1(e^{-iz}) + C\,\mathrm{Li}_1^{(1)}(e^{iz}) + D\,\mathrm{Li}_1^{(1)}(e^{-iz}), \tag{93}$$

where the absolute constants are

$$A := \frac{1}{4} + \frac{1}{2\pi i}(\gamma + \log 2\pi),\; C := -\frac{1}{2\pi i},\; B := A^*,\; D := C^*. \tag{94}$$

Here $'*'$ denotes the complex conjugate. We define a vector space $\mathcal{V}_1$ whose basis is $\mathcal{D}_1$, with coefficients generated by the rationals $\mathcal{Q}$ and four fundamental constants $\{\pi, \frac{1}{\pi}, \gamma, g := \log 2\pi\}$. 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 integrals

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

As foreshadowed in [4]:

Theorem 11. *For integer $n \geq 0$, the log-gamma integral is resolvable in that $\mathcal{L}G_n \in \mathcal{V}_1$.*[2]

[2]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,

$$\mathcal{G}_n := \int_0^1 \left(\log\Gamma(z) - \frac{g}{2}\right)^n dz \tag{95}$$

is in $\mathcal{V}_1$, because it is a classic Eulerian result that $\mathcal{L}G_1 = \frac{g}{2}$ (i.e. $G_1 = 0$), so that for $n > 1$ we may use recursion in the ring to resolve $\mathcal{L}G_n$. By formula (93), we write $\mathcal{G}_n$ as

$$\mathcal{G}_n := n! \sum_{a+b+c+d=n} \frac{A^a B^b C^c D^d}{a!b!c!d!} \mathcal{U}(a+c, b+d, c, d),$$

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

Example 6 (Examples of $\mathcal{G}$)**.** For $n = 1$, we have Euler's evaluation [4]

$$\mathcal{G}_1 = \int_0^1 \left(\log\Gamma(z) - \frac{g}{2}\right) dz = 0. \tag{96}$$

For $n = 2$ and $n = 3$ these evaluations lead to those previously published in [4]. For $n = a+b+c+d = 4, 5, 6\ldots$ we extract previously unresolved evaluations. For instance,

(97)

$$\begin{aligned}
\mathcal{G}_5 &= \int_0^1 \left(\log\Gamma(z) - \frac{g}{2}\right)^5 dz \\
&= \frac{5\left(4h^2+\pi^2\right)^2}{256\pi^4}\mathcal{U}(3,2,0,0) - \frac{5h\left(4h^2+\pi^2\right)}{16\pi^4}\mathcal{U}(3,2,0,1) \\
&+ \frac{15\left(4h^2+\pi^2\right)}{32\pi^4}\mathcal{U}(3,2,1,1) - \frac{15\left(4h^2+\pi^2\right)}{64\pi^4}\mathcal{U}(3,2,2,0) \\
&+ \frac{5\left(\pi^2-12h^2\right)\left(4h^2+\pi^2\right)}{512\pi^4}\mathcal{U}(4,1,0,0) + \frac{5h\left(4h^2+\pi^2\right)}{16\pi^4}\mathcal{U}(4,1,1,0) \\
&- \frac{15\left(4h^2+\pi^2\right)}{64\pi^4}\mathcal{U}(4,1,2,0) + \frac{5\left(12h^2-\pi^2\right)}{64\pi^4}\mathcal{U}(3,2,0,2) - \frac{15h}{8\pi^4}\mathcal{U}(3,2,1,2) \\
&+ \frac{5h}{8\pi^4}\mathcal{U}(3,2,3,0) + \frac{5\left(\pi^2-12h^2\right)}{32\pi^4}\mathcal{U}(4,1,1,1) + \frac{15h}{8\pi^4}\mathcal{U}(4,1,2,1) \\
&+ \frac{5h\left(4h^2-\pi^2\right)}{32\pi^4}\mathcal{U}(4,1,0,1) + \frac{15}{16\pi^4}\mathcal{U}(3,2,2,2) - \frac{5}{8\pi^4}\mathcal{U}(3,2,3,1) \\
&- \frac{5}{8\pi^4}\mathcal{U}(4,1,3,1) + \frac{5}{32\pi^4}\mathcal{U}(4,1,4,0).
\end{aligned}$$

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

$$\mathcal{U}(4,1,4,0) = \omega\left(\begin{array}{c|c} 1,1,1,1 & 1 \\ 1,1,1,1 & 0 \end{array}\right) = \sum_{m,n,p,q} \frac{\log m \, \log n \, \log p \, \log q}{m\,n\,p\,q\,(m+n+p+q)} \tag{98}$$

and the double MTW sum:

$$\mathcal{U}(3,2,3,0) = \omega\left(\begin{array}{c|c} 1,1,1 & 1,1 \\ 1,1,1 & 0,0 \end{array}\right) = \sum_{m,n,p,q}{}' \frac{\log m \, \log n \, \log p}{m\,n\,p\,q\,(m+n+p-q)}. \tag{99}$$

Here the '′' indicates we avoid the poles. It is a triumph of the integral representations that these very slowly convergent sums (of weight nine and eight respectively) can be calculated to extreme precision in short time. ♢

Remark 2. In all the examples above $\pi^{n-1}\mathcal{LG}_N$ is realized with no occurrence of $1/\pi$; with more care it should be possible to adduce this in the proof of Theorem 11. ♢

6.2. **An exponential generating function for the $\mathcal{LG}_n$.** To conclude this analysis, we again turn to generating functions. Let us define:

$$\mathcal{Y}(x) := \sum_{n\geq 0} \mathcal{L}G_n \frac{x^n}{n!} \;=\; \int_0^1 \Gamma^x(1-t)\,\mathrm{d}t. \tag{100}$$

Now, from the exponential series form for Γ given in (23), we obtain

Theorem 12. *For* $n = 1, 2, \ldots$

$$\mathcal{L}G_n \;=\; \sum_{m_1,\ldots,m_n\geq 1} \frac{\zeta^*(m_1)\,\zeta^*(m_2)\cdots\zeta^*(m_n)}{m_1 m_2\cdots m_n(m_1+\ldots m_n+1)}, \tag{101}$$

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

In particular, Euler's evaluation of $\mathcal{L}G_1$ 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 $\mathcal{L}G_n$ can be finite superpositions of *derivative* MTWs, and yet for any n these log-gamma integrals as infinite sums engage only 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 constants and functions being analyzed, we performed several numerical computations.

7.1. **Computations of the $\mathcal{G}$ constants.** Our first computation obtained $\mathcal{G}(2)$, $\mathcal{G}(3)$, $\mathcal{G}(4)$ and $\mathcal{G}(5)$ to 400-digit precision, using *Mathematica* and the integral formulas above. Then we separately computed these constants using closed forms such as (97). This second set of computations was performed with a combination of the ARPREC arbitrary precision software [7] and our implementation of tanh-sinh quadrature (74) to find the numerous $\mathcal{U}$ constants that appear in formulas such as (97). We employed formulas (45), (46), (53) and (55) to evaluate the underlying polylog and polylog derivatives; and formulas (56), (57), (59), (60) and (61) to evaluate the underlying zeta and zeta derivatives.

The results of these two sets of calculations matched to 400-digit accuracy.

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 $\mathcal{D}_1$ 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 program found that there are 149 constants in this class.

These computations, as above, were performed using the ARPREC arbitrary precision software [7] and the tanh-sinh quadrature algorithm (74), employing formulas (45), (46), (53) and (55) to evaluate the underlying polylog and polylog derivatives; and formulas (56), (57), (59), (60) and (61) 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 [6], [12, pp. 230–234]. Our program first found the following relations, confirmed to over 3000-digit precision:

$$0 = \mathcal{U}(M, M, p, q) - \mathcal{U}(M, M, q, p), \tag{102}$$

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

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

$$\begin{aligned}
0 &= 6\mathcal{U}(2,2,0,0) - 11\mathcal{U}(3,1,0,0),\\
0 &= 160\mathcal{U}(3,3,0,0) - 240\mathcal{U}(4,2,0,0) + 87\mathcal{U}(5,1,0,0),\\
0 &= 1680\mathcal{U}(4,4,0,0) - 2688\mathcal{U}(5,3,0,0) + 1344\mathcal{U}(6,2,0,0) - 389\mathcal{U}(7,1,0,0),\\
0 &= 32256\mathcal{U}(5,5,0,0) - 53760\mathcal{U}(6,4,0,0) + 30720\mathcal{U}(7,3,0,0),\\
&\quad - 11520\mathcal{U}(8,2,0,0) + 2557\mathcal{U}(9,1,0,0).
\end{aligned} \tag{103}$$

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

The entire computation, including quadrature and PSLQ calculations, required 94,727 seconds run time on one core of a 2012-era Apple *MacPro* workstation. Of this run time, initialization (including the computation of zeta and zeta derivative values, 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 [8]) 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).

These relations can be established by using *Maple* to symbolically evaluate the right-hand 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 (103). Similarly, the third relation in (103) follows from

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

7.3. **A conjecture posited, then proven.** From the equations in (103) we *conjectured* that: (i) there is one such relation at each even weight $(4,6,8,\ldots)$ and none at odd weight, and (ii) in each case $p=q=0$. Thus, there appear to be no nontrivial relations between derivatives outside $\mathcal{D}_0$ but in $\mathcal{D}_1$. Any negative results must perforce be empirical as one cannot at the present prove things even as "simple" as the irrationality of $\zeta(5)$. Accordingly, we performed a second computation: using 780-digit arithmetic and only computing elements of a given weight d, where $4 \le d \le 20$, with $m+n=d$ and $p=q=0$. The PSLQ search then quickly returned the additional relations culminating with:

$$\begin{aligned}
0 = &-698880340787 20\,\mathcal{U}(9,9,0,0) + 125798461341696\,\mathcal{U}(10,8,0,0)\\
&- 91489790066688\,\mathcal{U}(11,7,0,0) + 53369044205568\,\mathcal{U}(12,6,0,0)\\
&- 24631866556416\,\mathcal{U}(13,5,0,0) + 8797095198720\,\mathcal{U}(14,4,0,0)\\
&- 2345892052992\,\mathcal{U}(15,3,0,0) + 439854759936\,\mathcal{U}(16,2,0,0)\\
&- 51747618627\,\mathcal{U}(17,1,0,0),\\
0 = &-14799536744824832\,\mathcal{U}(10,10,0,0) + 26908248626954240\,\mathcal{U}(11,9,0,0)\\
&- 20181186470215680\,\mathcal{U}(12,8,0,0) + 12419191673978880\,\mathcal{U}(13,7,0,0)\\
&- 6209595836989440\,\mathcal{U}(14,6,0,0) + 2483838334795776\,\mathcal{U}(15,5,0,0)\\
&- 776199479623680\,\mathcal{U}(16,4,0,0) + 182635171676160\,\mathcal{U}(17,3,0,0)\\
&- 30439195279360\,\mathcal{U}(18,2,0,0) + 3204125819155\,\mathcal{U}(19,1,0,0).
\end{aligned} \tag{104}$$

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

Remark 3. As noted 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 nonzero.

Along the same lines, a natural and fairly accessible computational experiment would venture further outside of $\mathcal{D}_1$, motivated by (79). Any exhaustive study of the ensemble $\mathcal{D}$ is impractical pending a reliable arbitrary-precision implementation of high-order derivatives for $\mathrm{Li}_s(x)$ with respect to s. Hence, in light of (80), (81) and (82) it makes sense to hunt for relations of weight at most 20 with total derivative weight 2, say.

This study has underscored the need for high-precision evaluations of special functions in such research. This 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 [20]. Since, as we have illustrated, the polylogarithms and their relatives are central to a great deal of mathematics and mathematical physics [3, 15, 26], 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:

$$\omega(s_1,\ldots,s_{50} \mid t_1,\ldots,t_{50}) := \sum_{\substack{m_1,\ldots,m_{50},n_1,\ldots,n_{50}>0 \\ \sum_{i=1}^{50} m_i = \sum_{j=1}^{50} n_j}} \prod_{i=1}^{50} \frac{1}{{m_i}^{s_i}} \prod_{j=1}^{50} \frac{1}{{n_j}^{t_j}}. \tag{105}$$

We challenge readers to directly evaluate this sum.

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Lawrence Berkeley National Laboratory, Berkeley, California 94720
E-mail address: DHBailey@lbl.gov

CARMA, University of Newcastle, Callaghan, NSW 2308, Australia and Distinguished Professor King Abdulaziz University, Jeddah
E-mail address: jonathan.borwein@newcastle.edu.au

Center for Advanced Computation, Reed College, Portland, Oregon 97202
E-mail address: crandall@reed.edu