Extended Mordell-Tornheim-Witten sums and log Gamma integrals

D.H. Bailey, J.M. Borwein and R.E. Crandall

CARMA, University of Newcastle

TALK http://www.carma.newcastle.edu.au/jon/MTW1G.pdf
PAPER http://www.carma.newcastle.edu.au/jon/MTW1.pdf

Aust MS 2012, Ballarat, Number Theory Session

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A first obligatory irrelevant cartoon

A second obligatory irrelevant cartoon

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).

- We use symbolic and high-precision numerical integration, plus some interesting combinatorics and special- function theory.
- Our original motivation was to represent unresolved constructs such as Eulerian log-gamma integrals.
- In process, we extend methods for high- precision numerical computation of polylogarithms and their derivatives wrt order.

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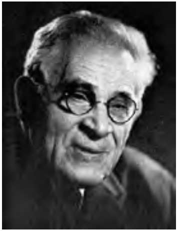
Coauthors (Lawrence Berkeley Labs and Apple Computers)

David Bailey

Richard Crandall

Mordell, Tornheim and Witten



HARMONIC DOUBLE SERIES.*

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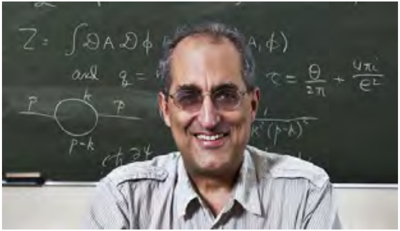

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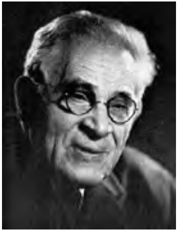

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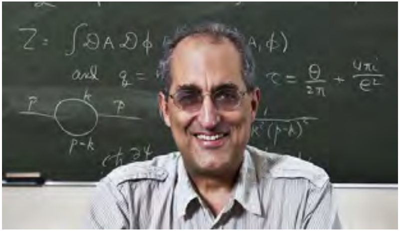

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Outline of Lecture: we will touch on some of

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We define an ensemble of extended Mordell–Tornheim –Witten (MTW) zeta function values.

- 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 deeper connections with multiple-zeta values (MZVs).
- To achieve this we make use of symbolic and numerical integration, special function theory and some less-than-obvious combinatorics and generating function analysis.

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Introduction

- Our original motivation was that of representing previously unresolved constructs such as Eulerian log-gamma integrals.
- Indeed, an algebra of MTW sums with constants $\pi, 1/\pi, \gamma, \log 2\pi$ and rationals, resolves every integral

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

(a finite superposition of MTW values with such coefficients).

- That said, our focus is the relation between MTW sums and classical polylogarithms. It is the adumbration of this relationship that makes the study significant.

PART I.

- We introduce an ensemble $\mathcal{D}$ capturing the values we wish to study and provide effective integral representations in terms of polylogarithms on the unit circle.
- We then identify subensemble $\mathcal{D}_1$ sufficient for study of log-gamma integrals; we give a few accessible closed forms.
- §3 give generating functions for various derivative free MTW sums and proves results suggested by experiments.
- §4 gives polylogarithmic algorithms for computation of our sums/integrals to high precision (400–3100 digits).
- We must first give tools for zeta and its derivatives at integer points. These are of substantial independent value.

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PART II

- §5 gives various reductions and relations of our MTW values.
- §6, shows how to evaluate all log gamma integrals $\mathcal{LG}_n$ for $n = 1, 2, 3\ldots$, in our special ensemble of MTW values.
- The associated paper describes two *rigorous experiments* we designed to use *integer relation methods* to first explore the structure of $\mathcal{D}_1$ and to begin to study $\mathcal{D}$ (mainly open).

My ugliest picture: an Australian blob fish

The Mordell–Tornheim–Witten (MTW) zeta function:

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

— ω remains mysterious for many combinatorial phenomena, especially for derivatives wrt the s_i parameters. (Here $K+1$ is the *depth* and $\sum_{j=1}^{k+1} s_j$ is the *weight* of ω. Originally $K=2$.)

We recently used a double sum with integers M, N and $s_i, t_j \geq 0$ $(M \geq N \geq 1)$ (here $\mathrm{Li}_s(z) := \sum_{n\geq 1} z^n/n^s$ is *polylogarithm of order s*):

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

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

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Generalized MTW ensembles

- If parameters are zero, there are convergence issues with this integral. One may use principal-value calculus, or an alternative representation such as (11) below.
  - when $N = 1$ the representation (3) is classical, in that

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

We require a wider *MTW ensemble* involving outer derivatives:

$$\omega\begin{pmatrix} s_1,\ldots,s_M & | & t_1,\ldots,t_N \\ d_1,\ldots,d_M & | & e_1,\ldots e_N \end{pmatrix} := \sum_{\substack{m_1,\ldots,m_M,n_1,\ldots,n_N>0 \\ \sum_{i=1}^M m_i=\sum_{j=1}^N n_j}} \prod_{i=1}^M \frac{(-\log m_i)^{d_i}}{{m_i}^{s_i}} \prod_{j=1}^N \frac{(-\log n_j)^{e_j}}{{n_j}^{t_j}}$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \prod_{i=1}^M \mathrm{Li}_{s_i}^{(d_i)}\left(e^{i\theta}\right) \prod_{j=1}^N \mathrm{Li}_{t_j}^{(e_j)}\left(e^{-i\theta}\right) d\theta, \tag{5}$$

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

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- 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:

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

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Important subensembles

We define $\mathcal{U}(m,n,p,q)$ to vanish if $mn = 0$; else if $m \geq n$ then

$$\mathcal{U}(m,n,p,q) := \frac{1}{2\pi}\int_0^{2\pi} \mathrm{Li}_1\left(e^{i\theta}\right)^{m-p} \mathrm{Li}_1^{(1)}\left(e^{i\theta}\right)^{p} \mathrm{Li}_1\left(e^{-i\theta}\right)^{n-q} \mathrm{Li}_1^{(1)}\left(e^{-i\theta}\right)^{q} \,\mathrm{d}\theta$$
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while for $m < n$ we swap both (m,n) and (p,q). We then denote

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

and $\mathcal{D}_0 \subset \mathcal{D}_1 \subset \mathcal{D}$ is a *derivative-free* set of MTWs

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

that is an element of $\mathcal{D}_0$ has the form $\omega(\mathbf{1}_M \mid \mathbf{1}_N)$. Likewise

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

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First (elementary) closed forms

For $N = 1$ in definition (5) we have the following:

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

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

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

- $\zeta(s, r)$ is a *multiple-zeta value* (MZV), some of which — such as $\zeta(6, 2)$ — are unresolved and are believed *irreducible*.

For the classic MTW (1), there is a useful pure-real integral available as an alternative to integral representation (3). In fact,

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

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Eqn. (11) can be split into a series plus a numerically easier incomplete Gamma integral With a free parameter λ, one has

$$\omega(s_1, s_2, \ldots, s_M \mid t) = \frac{1}{\Gamma(t)} \int_0^\lambda x^{t-1} \prod_{j=1}^M \mathrm{Li}_{s_j}(e^{-x})\,\mathrm{d}x \qquad (12)$$

$$+ \frac{1}{\Gamma(t)} \sum_{m_1,\ldots,m_M \geq 1} \frac{\Gamma(t, \lambda(m_1 + \cdots + m_M))}{m_1^{s_1} \cdots m_M^{s_M}\ (m_1 + m_2 + \cdots m_M)^t},$$

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

- There are interesting symbolic uses of (11): since $\mathrm{Li}_0(z) = \frac{z}{1-z}$,

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

- MZV Analytic continuation is known to be nontrivial. The continuation for $t \to 0$ appears to be $\omega(0,0,0,0 \mid 0) \stackrel{?}{=} \frac{251}{720}$, but the zeta-product formula (9) gives $\omega(0,0,0,0 \mid 0) = \zeta(0)^4 \stackrel{?}{=} \frac{1}{16}$.

First (elementary) closed forms

Eqn. (11) can be split into a series plus a numerically easier incomplete Gamma integral With a free parameter λ, one has

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

$$+ \frac{1}{\Gamma(t)} \sum_{m_1,\ldots,m_M \geq 1} \frac{\Gamma(t, \lambda(m_1 + \cdots + m_M))}{m_1^{s_1} \cdots m_M^{s_M}\ (m_1 + m_2 + \cdots m_M)^t},$$

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Resolution of all $\mathcal{U}(m,n)$

- There is an important class of resolvable MTWs where N is allowed to roam freely.
- Consider $\mathcal{D}_0$ from §2: the MTW is derivative-free with all ones across the top row.

The following experimentally motivated results provide an elegant generating function for $\mathcal{U}(m,n) := \mathcal{U}(m,n,0,0)$.

Theorem (Generating function $\mathcal{V}$ for $\mathcal{U}(m,n)$ as in (7))

We have

$$\mathcal{V}(x,y) := \sum_{m,n\geq 0} \mathcal{U}(m,n)\,\frac{x^m\,y^n}{m!\,n!} = \frac{\Gamma(1-x-y)}{\Gamma(1-x)\Gamma(1-y)}. \qquad (13)$$

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Proof.

Starting with the integral form in (7), we exchange integral and summation and then an obvious change of variables to arrive at

$$\mathcal{V}(x,y) = \frac{2^{-x-y+1}}{\pi}\int_0^{\pi/2} (\cos\theta)^{-x-y}\cos\left((x-y)\,\theta\right)\,\mathrm{d}\theta. \tag{14}$$

Using the beta function, for Re $a>0$ [DLMF, (5.12.5)] is:

$$\int_0^{\pi/2} (\cos\theta)^{a-1}\cos(b\theta)\,\mathrm{d}\theta = \frac{\pi}{2^a}\frac{1}{a\,\mathrm{B}\left(\frac{1}{2}(a+b+1),\frac{1}{2}(a-b+1)\right)}. \tag{15}$$

On setting $a=1-x-y, b=x-y$ in (15) we obtain (13). □

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Setting $y = \pm x$ in (13) leads to two natural one-dimensional generating functions. For instance

$$\mathcal{V}(x,-x) = \sum_{m,n\geq 1} (-1)^n \binom{m+n}{n} \mathcal{U}(m,n) \frac{x^{m+n}}{(m+n)!} = \frac{\sin(\pi x)}{\pi x}. \tag{16}$$

- Theorem 1 makes it very easy to evaluate $\mathcal{U}(m,n)$ symbolically in *Maple*. For instance, $\mathcal{U}(5,5)$ returns:

$$9600\,\pi^2\zeta(5)\,\zeta(3) + 600\,\zeta^2(3)\,\pi^4 + \frac{77587}{8316}\,\pi^{10} + 144000\,\zeta(7)\,\zeta(3) + 72000\,\zeta^2(5) \tag{17}$$

  - on a current *Lenovo* in a fraction of a second. The 61 terms of $\mathcal{U}(12,12)$ took 1.31 secs and the 159 terms for $\mathcal{U}(15,15)$ took 14.71 secs. To 100 digits it is

$$8.810791818778736904649020672776766667353256223589929081929162096395561049543747340201380539725128849 \times 10^{31}. \tag{18}$$

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They have been considered by Lewin, and recently used in QFT.

Lewin's result can be restated as

$$\mathcal{L}(x,y) := \sum_{m,n=0}^{\infty} 2^{m+n}\mathcal{B}Lsc_{m+1,n+1}(\pi)\,\frac{x^m}{m!}\,\frac{y^n}{n!}$$

$$= \pi\binom{2x}{x}\binom{2y}{y}\frac{\Gamma(1+x)\,\Gamma(1+y)}{\Gamma(1+x+y)}. \qquad (20)$$

This is closely linked to (13). Indeed, we may rewrite (20) as

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A generating function for $\mathcal{V}$

For a generating function $\mathcal{V}(x,y)$, we need expansions of the Gamma function. Recall the classical formulas

$$\log\Gamma(1-z) = \gamma z + \sum_{n>1}\zeta(n)\frac{z^n}{n}, \tag{22}$$

$$e^{-\gamma z}\Gamma(1-z) = \exp\left\{\sum_{n>1}\frac{\zeta(n)z^n}{n}\right\},$$

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

This leads immediately to a powerful representation for $\mathcal{V}$:

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Complete resolution of the ensemble $\mathcal{D}_0$

We may now read off values of $\mathcal{U}(m,n)$:

Theorem (Thm 2. Evaluation of $\mathcal{U}(M,N)$ for $M \geq N \geq 1$)

$\mathcal{U}(M,N) = \omega(\mathbf{1}_M \mid \mathbf{1}_N) \in \mathcal{D}_0$ *lies in the ring generated as*

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

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

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

Resolution of the ensemble $\mathcal{D}_0$

Proof.

Denote by Q the quantity in the braces $\{\ \}$ of the exponent in (23). Then inspection of

$$\exp\{Q\} = 1 + Q + Q^2/2! + \ldots$$

gives the finite form for a coefficient $\mathcal{U}(m,n)$. □

Example (Sample $\mathcal{U}$ values (all of weight $m+n$))

$$\mathcal{U}(4,2) = \omega(1,1,1,1\,|1,1) = 204\,\zeta(6) + 24\,\zeta(3)^2,$$

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Sum rule for $\mathcal{U}(m,n)$

Extreme-precision experiments discovered a unique sum rule amongst $\mathcal{U}$ functions with a fixed *even* order $M+N$. Eventually, with B_p the p-th Bernoulli number, we were led to:

Theorem (Sum rule for $\mathcal{U}$ of even weight $p>2$)

$$\sum_{m=2}^{p-2}(-1)^m\binom{p}{m}\mathcal{U}(m,p-m) \;=\; 2p\left(1-\frac{1}{2^p(p+1)B_p}\right)\mathcal{U}(p-1,1) \tag{24}$$

Proof.

Equate powers of x on each side of $\mathcal{V}(x,-x)$ (relation (16)), and use $\mathcal{U}(p-1,1)=(p-1)!\,\zeta(p)$ together with the Bernoulli form of $\zeta(p)$ given in (62). □

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Sum rule for $\mathcal{U}(m,n)$

Example (Sum rule for weights $M+N=20,100$)

For $M+N=20$, the theorem gives *precisely* the relation first numerically discovered.

Empirically this 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}.*

Further conditions for ring membership

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

$$\omega(\mathbf{1}_a\,\mathbf{0}_b \mid c) \;=\; \frac{(-1)^{a+c-1}}{\Gamma(c)} \int_0^1 \frac{(1-u)^{b-1}}{u^b} \log^{c-1}(1-u) \log^a u \, du, \tag{25}$$

is finite and the a ones and b zeros can be permuted.

- Such integrals are covered by below, but their special form of (25) resolves entirely to sums of 1-dim zeta products.
- Partial derivatives of the beta function, $B_{a,c-1}$, lead to:

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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.

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Proof. From (25) we have, formally.

$$(-1)^{a+c-1}\Gamma(c)\,\omega(\mathbf{1}_a\,\mathbf{0}_b \mid c) = \lim_{u\to -b}\frac{\partial}{\partial v^{(c-1)}}\left\{\frac{\partial}{\partial u^a}\frac{\Gamma(u+1)\Gamma(v)}{\Gamma(u+v+1)}\right\}_{v=b}. \tag{26}$$

Expanding $(1-u)^{b-1}/u^b$ binomially, the ω value is a superposition of terms $I(a,b,c) :=$

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Thence, we obtain the asserted reduction via the exponential-series arguments of the previous section or by appealing to known properties of poly-gamma functions. □

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Further conditions for ring membership

- In [Lewin, (7.128)] one finds $I(2,1,2) = 8\,\zeta\,(5) - \frac{2}{3}\,\zeta\,(3)\,\pi^2$ and an incorrect value for $I(3,1,2) = 6\,\zeta^2\,(3) - \frac{1}{105}\,\pi^6$.

Example (Representative evaluations are)

$$\omega(1,1,1,0,0 \mid 3) = (\pi^2 - 12)\,\zeta(3) - 3\,\zeta(3)^2 - 18\,\zeta(5) + \pi^2 + \frac{\pi^4}{12} + \frac{\pi^6}{210} \tag{28}$$

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

Now, not all terms have the same weight.

The subensemble $\mathcal{D}_0(s)$ for $s = 1, 2, 3\ldots$

Given the success with $\mathcal{V}$ in §3, we turn to $\mathcal{D}_0(s)$ from §2. We set $\mathcal{U}_s(0,0) = 1$; $\mathcal{U}_s(m,n) = 0$ if $m > n = 0$; else if $m \geq n$ we set

$$\mathcal{U}_s(m,n) := \frac{1}{2\pi}\int_0^{2\pi} \mathrm{Li}_s\left(e^{i\theta}\right)^m \mathrm{Li}_s\left(e^{-i\theta}\right)^n \,\mathrm{d}\theta = \omega\left(\begin{array}{c|c} \mathbf{s}_m & \mathbf{s}_n \\ \mathbf{0}_m & \mathbf{0}_n \end{array}\right). \tag{30}$$

That is, we consider elements $\omega(\mathbf{s}_M \mid \mathbf{s}_N)$. An obvious identity is

$$\mathcal{U}_s(1,1) = \zeta(2s). \tag{31}$$

Likewise

$$\mathcal{U}_s(2,1) = \omega(s,s,s), \tag{32}$$

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Evaluation of $\mathcal{V}_2$

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

$$\mathcal{V}_2(x,y) := \sum_{m,n\geq 0} \mathcal{U}_2(m,n)\,\frac{x^m\,y^n}{m!\,n!}. \tag{33}$$

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

$$\mathcal{V}_2(ix,iy) := \frac{1}{2\pi}\int_0^{2\pi} e^{(y-x))\mathrm{Cl}_2(\theta)} \cos\left(\frac{\left(2\,\pi^2+3\,\theta^2-6\,\pi\,\theta\right)}{12}\,(y+x)\right)\,d\theta \tag{34}$$

$$+\,i\,\frac{1}{2\pi}\int_0^{2\pi} e^{(y-x))\mathrm{Cl}_2(\theta)} \sin\left(\frac{\left(2\,\pi^2+3\,\theta^2-6\,\pi\,\theta\right)}{12}\,(y+x)\right)\,d\theta$$

where $\mathrm{Cl}_2(\theta) := -\int_0^\theta \log\left(2\left|\sin\frac{t}{2}\right|\right)\,dt$ is the Clausen function.

Evaluation of $\mathcal{V}_2$

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

$$\mathcal{V}_2(x,y) := \sum_{m,n\geq 0} \mathcal{U}_2(m,n)\,\frac{x^m\,y^n}{m!\,n!}. \tag{33}$$

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

$$\mathcal{V}_2(ix,iy) := \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{(y-x))\mathrm{Cl}_2(\theta)} \cos\left(\frac{\left(2\,\pi^2+3\,\theta^2-6\,\pi\,\theta\right)}{12}\,(y+x)\right)\,\mathrm{d}\theta \tag{34}$$

$$+\,i\,\frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{(y-x))\mathrm{Cl}_2(\theta)} \sin\left(\frac{\left(2\,\pi^2+3\,\theta^2-6\,\pi\,\theta\right)}{12}\,(y+x)\right)\,\mathrm{d}\theta$$

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.

The evaluation of $\mathcal{V}_2$

- It seems daunting to place this in closed form, but we can evaluate $\mathcal{V}_2(x,x)$.

It transpires, in terms of the *Fresnel integrals* S and C [DLMF, §7.2(iii)], to be

$$2\pi\,\mathcal{V}_2(ix,ix) = \; 2\sqrt{\frac{\pi}{x}}\left(\cos\left(\frac{x\pi^2}{6}\right)C\left(\sqrt{\pi x}\right)+\sin\left(\frac{x\pi^2}{6}\right)S\left(\sqrt{\pi x}\right)\right) \tag{35}$$

$$+i\,2\sqrt{\frac{\pi}{x}}\left(\cos\left(\frac{x\pi^2}{6}\right)S\left(\sqrt{\pi x}\right)-\sin\left(\frac{x\pi^2}{6}\right)C\left(\sqrt{\pi x}\right)\right).$$

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Series representations in [DLMF, Eq. (7.6.4) & (7.6.6)] give:

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

and

$$\mathrm{Im}\ \mathcal{V}_2(ix,ix) = -\sin\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^{\infty}\frac{(-1)^n\,\pi^{4n}}{2^{2n+2}\,(2n)!\,(4n+1)}\,x^{2n} + \cos\left(\frac{x\pi^2}{6}\right)\sum_{n=0}^{\infty}\frac{(-1)^n\,\pi^{4n+2}}{2^{2n+3}\,(2n+1)!\,(4n+3)}\,x^{2n+1}. \qquad (37)$$

The evaluation of $\mathcal{V}_2$

- $\mathrm{Re}\mathcal{V}_2(ix,ix)$ is an even function and $\mathrm{Im}\mathcal{V}_2(ix,ix)$ is odd.

On comparing (33) with $ix = iy$ to (36) or (37) we arrive at:

Theorem (Sum rule for $\mathcal{U}_2$)

For integer $p \geq 1$, there are explicit positive rationals q_p such that

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

$$\sum_{m=1}^{2p} \binom{2p+1}{m} \mathcal{U}_2(m, 2p+1-m) = (-1)^p\, q_{2p+1}\, \pi^{4p+2}. \tag{39}$$

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Example (Relations with $s = 2$)

Unlike $s = 1$ we have a relation of each weight for all even s.
The q_n are easy to compute from (35). Thence, to order 16:

$$\mathcal{V}_2(ix,ix) = -\frac{1}{90}\pi^4 x^2 + \frac{1}{22680}\pi^8 x^4 - \frac{53}{525404880}\pi^{12} x^6 + \frac{19}{128619114624}\pi^{16} x^8 \quad (40)$$

$$-\frac{1}{2835}\pi^6 x^3 + \frac{1}{561330}\pi^{10} x^5 - \frac{1}{262702440}\pi^{14} x^7 + \cdots . \quad (41)$$

Exact formulas for the coefficients of (40) are in (47) and (48) below.

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Remark

There is additional useful information to be gleaned from (34). Setting $y=-x$, we deduce that

$$\mathcal{V}_2(ix,-ix) = \frac{1}{\pi}\int_0^\pi \cos\left(\mathrm{Cl}_2(\theta)\,2x\right)\,\mathrm{d}\theta. \tag{42}$$

Comparing coefficients , 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 n.

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The evaluation of $\mathcal{V}_3$

- It is possible to undertake the same analysis generally.

For instance, from the evaluation Gl_3 we deduce that

$$\mathcal{V}_3(x,-x) = \frac{1}{\pi}\int_0^\pi \cos\left(\left(\pi^2-\theta^2\right)\frac{\theta}{6}\,x\right)\,\mathrm{d}\theta. \tag{43}$$

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 (31).
- Note also that $6\,\mathcal{U}_3(2,1)$ is the next coefficient and that all terms have the weight one would predict.

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The evaluation of $\mathcal{V}_N$

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:

$$\mathrm{Gl}_n(\theta) = (-1)^{1+\lfloor n/2 \rfloor} 2^{n-1} \frac{\pi^n}{n!} B_n\left(\frac{\theta}{2\pi}\right) \qquad (44)$$

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

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

The evaluation of $\mathcal{V}_N$

We then observe that:

$$\mathcal{V}_{2n+1}(x,-x) = \frac{1}{2\pi}\int_0^{2\pi} \cos\left(\mathrm{Gl}_{2n+1}\left(e^{i\theta}\right)x\right)\,\mathrm{d}\theta, \tag{45}$$

$$\mathcal{V}_{2n}(ix,ix) = \frac{1}{2\pi}\int_0^{2\pi} \exp\left(i\left(\mathrm{Gl}_{2n}\left(e^{i\theta}\right)x\right)\right)\,\mathrm{d}\theta. \tag{46}$$

- In each case substitution of (44) and term-by-term expansion of $\cos$ or $\sin$ leads to an expression for the coefficients
  - $\mathrm{Gl}_n(\theta)$ is an homogeneous two-variable polynomial in π and θ with each monomial of degree n

Indeed, we are thus led to the following explicit formulas:

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Indeed, we are thus led to the following explicit formulas:

The evaluation of $\mathcal{V}_N$

The real and imaginary coefficients of order $2m$ are respectively:

$$r_m(s) := (-1)^m \frac{4^{m-1}}{(2m)!\,\pi} \int_0^{2\pi} \left(\frac{(-1)^{1+\lfloor s/2 \rfloor}}{s!} (2\pi)^s B_n\left(\frac{\theta}{2\pi}\right)\right)^{2m} \mathrm{d}\theta \tag{47}$$

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Thence, we have established:

Theorem (Sum relations for $\mathcal{U}_s$)

Let s be a positive integer.

There is an analogue of Theorem 4 (the sum rule via $\mathcal{V}$) when s is odd and of Theorem 8 (sum rule via $\mathcal{V}_2$) when s is even.

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Fundamental computational expedients

To numerically study the ensemble $\mathcal{D}$ intensively, we must be able to differentiate polylogarithms with respect to their order.

- Even our primary goal herein—the study of $\mathcal{D}_1$—needs access to the first derivative of

$$\mathrm{Li}_1(x) = -\log(1-x)$$

(a derivative wrt one !).

- Below

$$H_n := 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n},$$

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Computing polylogarithms

When $s = n$ is a positive integer,

$$\mathrm{Li}_n(z) = {\sum_{m=0}^{\infty}}' \zeta(n-m)\frac{\log^m z}{m!} + \frac{\log^{n-1} z}{(n-1)!}\left(H_{n-1} - \log(-\log z)\right), \qquad (49)$$

valid for $|\log z| < 2\pi$. For any *order* s not a positive integer,

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$$\mathrm{Li}_s(z) := \sum_{k=1}^{\infty} \frac{z^k}{k^s}. \qquad (51)$$

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Computing polylogarithms

For integer k, $|\log z| < 2\pi$ and *all* $\tau \in [0,1)$ we have:

$$\mathrm{Li}_{k+1+\tau}(z) = \sum_{0\le n\ne k} \zeta(k+1+\tau-n)\frac{\log^n z}{n!} + \frac{\log^k}{k!}\sum_{j=0}^{\infty} c_{k,j}(\mathcal{L})\,\tau^j. \tag{52}$$

Here $\mathcal{L} := \log(-\log z)$ and $c_{k,j}$ engage the Stieltjes constants γ_j

$$c_{k,j}(\mathcal{L}) := \frac{(-1)^j}{j!}\gamma_j - b_{k,j+1}(\mathcal{L}), \tag{53}$$

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

$$b_{k,j}(\mathcal{L}) := \sum_{\substack{p+t+q=j\\ p,t,q\ge 0}} \frac{\mathcal{L}^p}{p!}\frac{\Gamma^{(t)}(1)}{t!}(-1)^{t+q} f_{k,q}. \tag{54}$$

Computing polylogarithms (This works really well)

Finally, $f_{k,q}$ is the coefficient of x^q in $\prod_{m=1}^{k} \frac{1}{1+x/m}$. The $f_{k,q}$ are easily calculable via $f_{k,0}=1$ and the recursion

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- To obtain first (or higher) derivatives $\mathrm{Li}_{k+1}^{(1)}(z)$, we differentiate (52) at zero and so require the evaluation $c_{k,1}$
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Computing polylogarithms with $s=1$ and $z=e^{i\theta}$

1. We may write, for $0<\theta\le 2\pi$,

$$\mathrm{Li}_1(e^{i\theta}) = -\log\left(2\sin\left(\frac{\theta}{2}\right)\right) + \frac{(\pi-\theta)}{2}i. \tag{56}$$

2. We saw 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

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

valid for $|\log z|<2\pi$. Here γ_1 is the *second Stieltjes constant*. For small $|z|$, it again suffices to use

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2. We saw 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

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

valid for $|\log z| < 2\pi$. Here γ_1 is the *second Stieltjes constant*. For small $|z|$, it again suffices to use

$$\mathrm{Li}_s'(z) = -\sum_{n=1}^{\infty}\frac{z^k \log k}{k^s}. \qquad (57)$$

Computing polylogarithms with $s = 1$ and $z = e^{i\theta}$

Hence

$$\mathrm{Li}_1'(e^{i\theta}) = \sum_{n=1}^{\infty} \zeta'(1-n)\,\frac{(i\theta)^n}{n!} - \gamma_1 - \frac{1}{12}\pi^2 - \frac{1}{2}\left(\gamma + \log(-i\theta)\right)^2, \tag{58}$$

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

- Note the bonus of being on the boundary of the disc!
- With such formulas, to evaluate $\mathcal{U}(m,n,p,q)$ one may use pure quadrature, convergent series, or a combination of both.
- All of these are gainfully exploited in computing MTW values.

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Computing zeta values (at integers)

- (49) or (56) and (50) or (58) require precomputed values of zeta and its derivatives at (often negative) integer arguments.
- One fairly efficient algorithm for computing a single $\zeta(n)$ for integer $n > 1$ is the following given by Peter Borwein:

Choose $N > 1.2 \cdot D$, where D is number of digits required. Then

$$\zeta(s) \approx -2^{-N}(1-2^{1-s})^{-1} \sum_{i=0}^{2N-1} \frac{(-1)^i \sum_{j=-1}^{i-1} u_j}{(i+1)^s}, \qquad (59)$$

where $u_{-1} = -2^N, u_j = 0$ for $0 \le j < N-1; u_{N-1} = 1$, and for $j \ge N$ compute

$$u_j = u_{j-1} \cdot (2N-j)/(j+1-N).$$

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Computing zeta values (at many integers)

- To obtain $\zeta(n)$ for many $n>1$, the following is more efficient.

First, to compute $\zeta(2n)$, observe that

$$\coth(\pi x) = -\frac{2}{\pi x}\sum_{k=0}^{\infty}\zeta(2k)(-1)^k x^{2k} = \frac{\cosh(\pi x)}{\sinh(\pi x)}$$
$$= \frac{1}{\pi x}\cdot\frac{1+(\pi x)^2/2!+(\pi x)^4/4!+(\pi x)^6/6!+\cdots}{1+(\pi x)^2/3!+(\pi x)^4/5!+(\pi x)^6/7!+\cdots}. \qquad (60)$$

Let $P(x), Q(x)$ be the numerator and denominator polynomials obtained by truncating these two series to n terms.

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Let $P(x), Q(x)$ be the numerator and denominator polynomials obtained by truncating these two series to n terms.

Computing even zeta values (by Newton's method)

Then the approximate reciprocal $R(x)$ of $Q(x)$ can be obtained by applying the Newton iteration

$$R_{k+1}(x) := R_k(x) + [1 - Q(x) \cdot R_k(x)] \cdot R_k(x). \qquad (61)$$

- Both polynomial degree and numeric precision of the coefficients are dynamically increased, doubling with each loop, until desired degree and precision are achieved. (FFT, FFT, FFT !)
- The quotient P/Q is now simply the product $P(x) \cdot R(x)$.
- The required values $\zeta(2k)$ can now be obtained from the coefficients of this product polynomial $P \cdot R$.

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Computing Bernoulli numbers (from even zeta values)

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

$$B_{2k} = (-1)^{k+1}\frac{2(2k)!}{(2\pi)^{2k}}\,\zeta(2k). \tag{62}$$

Zeta at odd positive integers (via Bernoulli numbers)

Positive odd-indexed zeta values can be now efficiently computed using Ramanujan-style hyperbolic corrections to Bernoulli sums:

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

$$\zeta(4N+1) = -\frac{1}{N}\sum_{k=1}^{\infty}\frac{(2\pi k+2N)\exp(2\pi k)-2N}{k^{4N+1}(\exp(2k\pi)-1)^2} - \frac{1}{2N}\pi(2\pi)^{4N}\sum_{k=1}^{2N+1}(-1)^k\frac{B_{2k}B_{4N+2-2k}}{(2k-1)!(4N+2-2k)!}. \qquad (63)$$

Computing zeta at negative integers

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

$$\zeta(-2n) = 0$$

and

$$\zeta(-2n+1) = -\frac{B_{2n}}{2n}. \qquad (64)$$

Computing derivatives of zeta at integers

- Precomputed values of the zeta derivative function are prerequisite for the efficient use of formulas (56) and (58).
- 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.
  - we use an adaptation of a scheme due to Crandall based on more general acceleration methods of Cohen-Villegas-Zagier:
    - in our algorithm, log and zeta values can be precalculated, and so do not significantly add to run time
    - similar techniques apply to higher derivatives of η—and so ζ—at positive integers.

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Computing ζ' at non-positive integers

From the functional equation for ζ:

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

one can extract

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

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

$$\zeta'(-m) := \frac{d}{ds}\zeta(s)|_{s=-m} \;=\; \frac{(-1)^{m/2}m!}{2^{m+1}\pi^m}\,\zeta(m+1), \qquad (65)$$

while for odd $m = 1, 3, 5\ldots,$

$$\zeta'(-m) \;=\; \zeta(-m)\left(\gamma \;+\; \log 2\pi \;-H_m - \frac{\zeta'(m+1)}{\zeta(m+1)}\right). \qquad (66)$$

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Derivatives of Γ at positive integers

- To approach ζ we first need to attack the Gamma function (one more efficient indirection).

Let $g_n := \Gamma^{(n)}(1)$. It is known [DLMF, (5.7.1) & (5.7.2)] that

$$\Gamma(z+1)\,\mathcal{C}(z) = z\,\Gamma(z)\,\mathcal{C}(z) = z \tag{67}$$

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

$$(k-1)c_k = \gamma c_{k-1} - \zeta(2)\,c_{k-2} + \zeta(3)\,c_{k-3} - \cdots + (-1)^k\,\zeta(k-1)\,c_1. \tag{68}$$

Thus, differentiating (67) by Leibniz' formula, for $n \geq 1$ we have

$$g_n = -\sum_{k=0}^{n-1} \frac{n!}{k!}\,g_k\,c_{n+1-k}. \tag{69}$$

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More generally, for positive integer m we have

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

where $(z)_m := z(z+1)\cdots(z+m-1)$ is the rising factorial polynomial.

Letting $g_n(m) := \Gamma^{(n)}(m)$ so that $g_n(1) = g_n$, we may again apply the product rule to (70) and obtain

$$g_n(m) = -\sum_{k=0}^{n-1} \frac{n!}{k!}\, g_k(m)\, c_{n+1-k} + \frac{D_m^{n+1}}{n+1}. \tag{71}$$

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

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Indeed

$$D_m^n = \sum_{k=0}^{m-n} s\,(m, k+n)\,(k+1)_n\,(m-1)^k = (n+1)!\,(-1)^{m+n+1} s\,(m, 1+n). \tag{72}$$

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

$$\frac{g_n(m)}{n!} = -\sum_{k=0}^{n-1} \frac{g_k(m)}{k!}\, c_{n+1-k} + |s(m,1+n)| \tag{73}$$

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see [DLMF, (26.8.18)].

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

Theorem (Apostol, see DLMF (25.6.13) and (25.6.14))

For $n = 0, 1, 2, \ldots$, *with* $\kappa := -\log(2\pi) - \frac{1}{2}\pi i$ *we have finite sums:*

$$(-1)^k \zeta^{(k)}(1-2n) = \frac{2(-1)^n}{(2\pi)^{2n}} \sum_{m=0}^{k} \sum_{r=0}^{m} \binom{k}{m} \binom{m}{r} \mathrm{Re}(\kappa^{k-m})\, \Gamma^{(r)}(2n)\, \zeta^{(m-r)}(2n), \tag{75}$$

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In (73), (74) for $\Gamma^{(r)}(m)$ *only the initial conditions rely on* m

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Tanh-sinh quadrature (is amazingly flexible)

Given $h>0$, one such scheme is

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} f(g(t))g'(t)\,\mathrm{d}t \approx h\sum_{j=-N}^{N} w_j f(x_j), \qquad (77)$$

where the abscissas x_j and weights w_j are given by

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- Here N is chosen so that terms beyond N are "negligible'
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Tanh-sinh quadrature of $\mathcal{U}$ integrals

- For $\mathcal{U}$ constant calculations, we may integrate from 0 to π, then divide by π, if we integrate the real part of the integrand.
- We typically compute numerous $\mathcal{U}(m,n,p,q)$, so it is much faster to precompute polylog and derivative functions (sans exponents) at each abscissa point x_j.
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Reduction of classical MTW values and derivatives

We now return to our objects of central interest. Partial fraction manipulations allow one to relate partial derivatives of MTWs.

Theorem (Thm. 13. Reduction of classical MTW derivatives)

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

$$\delta(r,s,t) = \sum_{i=1}^{r} \binom{r+s-i-1}{s-1} \delta\left(i, 0, N-i\right) + \sum_{i=1}^{s} \binom{r+s-i-1}{r-1} \delta\left(0, i, N-i\right). \tag{80}$$

When $\delta = \omega$ this shows each classical MTW value is a finite positive integer combination of MZVs. Herein, we use the shorthand

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

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$$\delta(r,s,t) = \sum_{i=1}^{r} \binom{r+s-i-1}{s-1} \delta(i, 0, N-i) + \sum_{i=1}^{s} \binom{r+s-i-1}{r-1} \delta(0, i, N-i). \qquad (80)$$

When $\delta = \omega$ this shows each classical MTW value is a finite positive integer combination of MZVs. Herein, we use the shorthand

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

Reduction of classical MTW values and derivatives

We now return to our objects of central interest. Partial fraction manipulations allow one to relate partial derivatives of MTWs.

Theorem (Thm. 13. Reduction of classical MTW derivatives)

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Reduction of classical MTW values and derivatives

Proof.

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:

$$d(r, s, t-1) = d(r-1, s, t) + d(r, s-1, t) \tag{81}$$

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

Reduction of classical MTW values and derivatives

Example (The numerical techniques provide values of δ)

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

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

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

while

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

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

$$\omega_{1,0,1}(1,1,2) = 0.43097253394888316942248176511038963971077201581912157523 09\ldots$$

and

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

Note $\omega_{1,1,0}(1,1,2) = 2\,\omega_{1,1,0}(1,0,3)$ and $\omega_{1,0,1}(1,0,3) + \omega_{1,0,1}(0,1,3) = \omega_{1,0,1}(1,1,2)$ both in accord with Theorem 13.

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A PSLQ discovery proven

The algorithm PSLQ run on the above data predicted that

$$\zeta''(4) \stackrel{?}{=} 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2) - 2\,\omega_{1,0,1}(2,0,2), \quad (82)$$

which also validates our high-precision techniques.

Proof.

First $\omega_{1,1,0}(2,2,0) = \zeta'(2)^2$. Next the MZV reflection formula $\zeta(s,t) + \zeta(t,s) = \zeta(s)\zeta(t) - \zeta(s+t)$, yields $\zeta_{1,1}(s,t) + \zeta_{1,1}(t,s)$ $= \zeta'(s)\zeta'(t) - \zeta^{(2)}(s+t)$. Hence $2\omega_{1,0,1}(2,0,2) = 2\zeta_{1,1}(2,2)$ $= \zeta'(2)^2 - \zeta''(4)$. Since $\omega_{1,1,0}(2,0,2) = 2\omega_{1,0,1}(2,1,1)$ by Thm 13, our desired formula is $\zeta''(4) + 2\,\omega_{1,0,1}(2,0,2) = 4\,\omega_{1,1,0}(1,0,3)$ $+2\,\omega_{1,1,0}(2,0,2)$, which is equivalent to $\zeta'(2)^2 = \omega_{1,1,0}(2,2,0)$ $= 4\,\omega_{1,1,0}(1,0,3) + 2\,\omega_{1,1,0}(2,0,2)$—another easy case of Thm 13. □

- (82) shows less trivial derivative relations exist within $\mathcal{D}$ than in $\mathcal{D}_1$.

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Relations when $M \ge N \ge 2$

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

Theorem (Relations for general ω)

$$\sum_{k=1}^{N} \omega\left(\begin{array}{c|c} s_1,\ldots,s_M & t_1,\ldots,t_{k-1},t_k-1,t_{k+1},\ldots,t_N \\ d_1,\ldots,d_M & e_1,\ldots e_N \end{array}\right)$$
$$= \sum_{j=1}^{M} \omega\left(\begin{array}{c|c} s_1,\ldots,s_{j-1},s_j-1,s_{j+1},\ldots,s_M & t_1,\ldots,t_N \\ d_1,\ldots,d_M & e_1,\ldots e_N \end{array}\right). \quad (83)$$

When $N = 1, M = 2$ this is precisely (81). For general M and $N = 1$ there is a result like Theorem 13.

Complete reduction of MTW values when $N = 1$

When $N = 1$ we can use the prior theorem to show every MTW value (without derivatives) is a finite sum of MZV's.

The basic tool is the partial fraction

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

Theorem (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) *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.*

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Complete reduction of MTW values when $N = 1$

Proof.

(a) for integers $a_i > 0$ and $b_j \geq 0$ (with b_n large enough to assure convergence) define $N_j := n_1 + n_2 + \cdots n_j$ and set

$$\kappa(a_1,\ldots,a_n \mid b_1,\ldots,b_n) := \sum_{n_i>0} \frac{1}{\prod_{i=1}^n {n_i}^{a_i} \prod_{j=1}^n {N_j}^{b_j}}. \tag{84}$$

Thence $\kappa(a_1,\ldots,a_n \mid b_1) = \omega(a_1,\ldots,a_n \mid b_1)$. Noting κ is symmetric in the a_i, let $\overrightarrow{a}$ 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, we deduce

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

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We repeat this step until there are only $k-1$ non-zero entries. Each step is weight invariant. As repeated rearrangements leave the N_j terms invariant, we arrive at a superposition of sums of the form

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

The process assures each a_i is reduced to zero and so each final $b_j > 0$. In particular, we may start with κ so that $a_i > 0, b_j = 0$ except for $j = n$. This captures our ω sums and other intermediate structures. Part (b) follows from recent results in the MZV literature. □

Tsimura proves reduction for exactly our MTWs with $N = 1$.

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MTW resolution of the log-gamma problem

- As a serious example of our interest in MTW sums we shall show $\mathcal{D}_1$ from §2 resolves the log-gamma integral problem—in that every log-gamma integral $\mathcal{LG}_n$ lies in a specific algebra.

We start, with the Kummer series:

$$\log\Gamma(x) - \frac{1}{2}\log(2\pi) = -\frac{1}{2}\log\left(2\sin(\pi x)\right) + \frac{1}{2}(1-2x)\left(\gamma + \log(2\pi)\right) + \frac{1}{\pi}\sum_{k=2}^{\infty}\frac{\log k}{k}\sin(2\pi k x) \qquad (85)$$

for $0 < x < 1$.

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MTW resolution of the log-gamma problem

Wth a view toward polylogarithm representations, this can be satisfactorily rewritten as:

$$\log\Gamma\left(\frac{z}{2\pi}\right) - \frac{1}{2}\log 2\pi = A\,\mathrm{Li}_1(e^{iz}) + B\,\mathrm{Li}_1(e^{-iz}) + C\,\mathrm{Li}_1^{(1)}(e^{iz}) + D\,\mathrm{Li}_1^{(1)}(e^{-iz}), \tag{86}$$

where the absolute constants are

$$A := \frac{1}{4} + \frac{1}{2\pi i}(\gamma + \log 2\pi),\ C := -\frac{1}{2\pi i},\ B := A^*,\ D := C^*. \tag{87}$$

Here $'*'$ denotes the complex conjugate.

MTW resolution of the log-gamma problem

We define a vector space $\mathcal{VV}_1$ generated by the subensemble $\mathcal{D}_1$, with coefficients generated by the rationals $\mathcal{Q}$ and four constants:

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

Specifically,

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

where any sum therein is finite.

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

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MTW resolution of the log-gamma problem

As foreshadowed in our earlier paper:

Theorem

For every integer $n \geq 0$, the n-th log-gamma integral can be resolved in the sense that $\mathcal{LG}_n \in \mathcal{VV}_1$.

- The proof exhibits an computationally effective and explicit form for the requisite superposition $\sum c_i \omega_i$ for any n.

MTW resolution of the log-gamma problem

Proof.

Inductively, it is enough to show that generally

$$\mathcal{G}_n := \int_0^1 \left(\log\Gamma(z) - \frac{g}{2}\right)^n \, \mathrm{dz} \tag{88}$$

is in $\mathcal{VV}_1$, because of Euler's classic result that $\mathcal{LG}_1 = \frac{g}{2}$ (i.e., $\mathcal{G}_1 = 0$), so that for $n > 1$ we may use recursion in the ring to resolve $\mathcal{LG}_n$. By formula (86), we write

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

where $\mathcal{U}$ has been defined by (7). This finite sum is in $\mathcal{VV}_1$. □

MTW resolution of the log-gamma problem

For $n=2$, the generators in $\mathcal{D}_1$ have $a+b+c+d=2$, and we extract an algebra superposition for $\mathcal{LG}_2$ via

$$\mathcal{G}_2 = \int_0^1 \left(\log\Gamma(z) - \frac{g}{2}\right)^2 dz \tag{89}$$

$$= \frac{\left(4(g+\gamma)^2+\pi^2\right)}{8\pi^2}\mathcal{U}(1,1,0,0) - \frac{(2g+2\gamma)}{4\pi^2}(\mathcal{U}(1,1,0,1) + \mathcal{U}(1,1,1,0)) + \frac{\mathcal{U}(1,1,1,1)}{2\pi^2}.$$

Since $\mathcal{U}(1,1,0,0)=\zeta(2)$, $\mathcal{U}(1,1,0,1)=\mathcal{U}(1,1,1,0)=\zeta'(2)$, and $\mathcal{U}(1,1,1,1)=\zeta''(2)$, this decodes as $\mathcal{LG}_2 =$

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MTW resolution of the log-gamma problem

To clarify notation we show the final weight nine $\mathcal{U}$-value for $\mathcal{G}_5$

$$\mathcal{U}(4,1,4,0) = \omega\begin{pmatrix} 1,1,1,1 & | & 1 \\ 1,1,1,1 & | & 0 \end{pmatrix} = \sum_{m,n,p,q} \frac{\log m \, \log n \, \log p \, \log q}{m\,n\,p\,q\,(m+n+p+q)}. \tag{90}$$

and the weight eight double MTW sum:

$$\mathcal{U}(3,2,3,0) = \omega\begin{pmatrix} 1,1,1 & | & 1,1 \\ 1,1,1 & | & 0,0 \end{pmatrix} = \sum_{m,n,p,q}{}' \frac{\log m \, \log n \, \log p}{m\,n\,p\,q\,(m+n+p-q)}. \tag{91}$$

- It is a triumph of the forms that these very slowly convergent sums can be rapidly calculated to extreme precision.
- I stumbled upon $\mathcal{D}$ from Fourier analysis of Kummer's series. Notation is important!

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

Let us define:

$$\mathcal{Y}(x) := \sum_{n\geq 0} \mathcal{LG}_n \frac{x^n}{n!} \;=\; \int_0^1 \Gamma^x(1-t)\,\mathrm{d}t. \tag{92}$$

From the exponential-series form for Γ given in (22), it follows that the general log-gamma integral is expressible as follows

Theorem

For $n = 1, 2, \ldots$ we have the infinite sum representation

$$\mathcal{LG}_n \;=\; \sum_{m_1,\ldots,m_n\geq 1} \frac{\zeta^*(m_1)\,\zeta^*(m_2)\cdots\zeta^*(m_n)}{m_1 m_2\cdots m_n(m_1+\cdots+m_n+1)}, \tag{93}$$

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

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

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

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

$$= \frac{1}{2} + \gamma + \sum_{m\ge 2} \frac{\zeta(m)-1}{m(m+1)}.$$

This is a rapidly convergent rational zeta-series.

- It is fascinating—and not understood—how the higher $\mathcal{LG}_n$ can be finite superpositions of *derivative* MTWs, and yet as infinite sums engage only ζ-function convolutions as above.

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Open Issues

1. Further determine structure of $\mathcal{D}_1$
2. Determine structure of $\mathcal{D}$
   - This relies on implementing a fuller version of §4's methods
3. Find more closed forms
4. Eventually, develop a comprehensive package of computational tools for effective high precision computation of special functions

Key References

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