Odd Relatives of MZVs

ME Hoffman

Outline
Introduction
Quasi-Symmetric Functions
MtVs of Repeated and Even Arguments
Iterated Integrals and Alternating MZVs
Calculations and Conjectures
Depth 2 Results

Odd Relatives of Multiple Zeta Values

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Outline

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Introduction

For positive integers $a_1, \ldots, a_k$ with $a_1 > 1$ we define the corresponding multiple $t$-value (MtV) by

$$t(a_1, a_2, \ldots, a_k) = \sum_{n_1 > n_2 > \cdots > n_k \geq 1, \ n_i \text{ odd}} \frac{1}{n_1^{a_1} n_2^{a_2} \cdots n_k^{a_k}}.$$

Except for the specification that the $n_i$ are odd, this is just the usual definition of the multiple zeta value $\zeta(a_1, \ldots, a_k)$. We say $t(a_1, \ldots, a_k)$ has depth $k$ and weight $a_1 + \cdots + a_k$. MtVs of depth 1 are simply related to values of the Riemann zeta function:

$$t(a) = \sum_{n > 0 \text{ odd}} \frac{1}{n^a} = \zeta(a) - \sum_{n > 0 \text{ even}} \frac{1}{n^a} = (1 - 2^{-a}) \zeta(a). \quad (1)$$
While multiple zeta values (for depth \( \leq 2 \)) appear in the correspondence between Euler and Goldbach in the 1740s, \( t \)-values can only claim a history of 110 years. In 1906 N. Nielsen showed that

\[
\sum_{i=1}^{n-1} t(2i)t(2n - 2i) = \frac{2n - 1}{2},
\]

which parallels the result Euler gave for zeta values:

\[
\sum_{i=1}^{n-1} \zeta(2i)\zeta(2n - 2i) = \frac{2n + 1}{2}.
\]
MtVs vs. MZVs

It turns out that the theory of multiple $t$-values is in some ways directly parallel to that for multiple zeta values, and in other ways completely different. The MtVs share with the MZVs the “harmonic algebra” (AKA “stuffle”) multiplication, e.g., just as

$$\zeta(2)\zeta(3, 1) = \zeta(2, 3, 1) + \zeta(3, 2, 1) + \zeta(3, 1, 2) + \zeta(5, 1) + \zeta(3, 3)$$

we have

$$t(2)t(3, 1) = t(2, 3, 1) + t(3, 2, 1) + t(3, 1, 2) + t(5, 1) + t(3, 3).$$

From this (and equation (1)) follows, e.g.,

$$t\underbrace{(2, \ldots, 2)}_n = \frac{\pi^{2n}}{2(2n)!}, \quad \text{cf.} \quad \zeta\underbrace{(2, \ldots, 2)}_n = \frac{\pi^{2n}}{(2n + 1)!}.$$
Similarly one has

\[ t(4, \ldots, 4) = \frac{\pi^{4n}}{2^{2n}(4n)!}, \quad t(6, \ldots, 6) = \frac{3\pi^{6n}}{4(6n)!}, \]

which directly parallel

\[ \zeta(4, \ldots, 4) = \frac{2^{2n+1}\pi^{4n}}{(4n+2)!}, \quad \zeta(6, \ldots, 6) = \frac{6\pi^{6n}}{(6n+3)!}. \]

But in other ways MtVs differ markedly from MZVs. For MZVs one has the sum theorem: the sum of all MZVs of weight \( n \) and depth \( k \) is \( \zeta(n) \), regardless of \( k \). There seems to be nothing comparable for MtVs.
Also absent from the MtVs is an analogue of the MZV duality; while one has, for example, the relations $\zeta(2,1,1) = \zeta(4)$ and $\zeta(3,1,2) = \zeta(2,3,1)$, nothing like this exists for MtVs. Duality of MZVs comes from an iterated integral representation: for example,

$$\zeta(3, 2) = \int_0^1 \frac{dx_5}{x_5} \int_0^{x_5} \frac{dx_4}{x_4} \int_0^{x_4} \frac{dx_3}{1-x_3} \int_0^{x_3} \frac{dx_2}{x_2} \int_0^{x_2} \frac{dx_1}{1-x_1}$$

and the change of variable

$$(x_1, x_2, x_3, x_4, x_5) \rightarrow (1-x_5, 1-x_4, 1-x_3, 1-x_2, 1-x_1)$$

leads to the duality relation $\zeta(3, 2) = \zeta(2, 2, 1)$. The iterated integral representation of MZVs leads to a second algebra structure (shuffle product).
MtVs vs. MZVs cont’d

For MtVs there is an iterated integral representation, but it’s not nearly as nice; for example,

\[
t(3, 2) = \int_0^1 \frac{dx_5}{x_5} \int_0^{x_5} \frac{dx_4}{x_4} \int_0^{x_4} \frac{x_3 dx_3}{1 - x_3^2} \int_0^{x_3} \frac{dx_2}{x_2} \int_0^{x_2} \frac{dx_1}{1 - x_1^2}.
\]

The change of variable above doesn’t take an iterated integral of this form to another, and integrals of this form are not closed under the shuffle product of forms. Already one sees the consequences in weight 3: while for MZVs one has the first instance of duality

\[
\zeta(2, 1) = \zeta(3)
\]

(discovered by Euler and many others since), for MtVs one has

\[
t(2, 1) = -\frac{1}{2} t(3) + t(2) \log 2.
\]
MtVs and alternating MZVs

Nevertheless, the iterated integral representation for MtVs does lead to a formula expressing any MtV as a sum of alternating MZVs, e.g.,

\[
\zeta(3, 2) = \sum_{n_1 > n_2 \geq 1} \frac{(-1)^{n_1}}{n_1^3 n_2^2}, \quad \zeta(3, \bar{2}) = \sum_{n_1 > n_2 \geq 1} \frac{(-1)^{n_2}}{n_1^3 n_2^2}.
\]

Alternating or “colored” MZVs have been studied, at least by physicists, since they began to turn up in quantum field theory in the late 1980s. Thanks to the Multiple Zeta Value Data Mine project of Blümlein, Broadhurst and Vermaseren, extensive tables expressing alternating MZVs in terms of a (provisional) basis exist.
A conjecture

We have used these expressions to write out the $t$-values through weight 7. Thus, e.g.,

$$t(2, 1, 3) = \frac{27}{112} t(6) - \frac{5}{28} t(3)^2 + \frac{1}{2} t(2) \zeta(\bar{3}, 1).$$

Calculations using these tables have led us to the following conjecture.

**Conjecture**

*The dimension of the rational vector space spanned by MtVs of weight $n \geq 2$ is $F_n$, the $n$th Fibonacci number.*

The corresponding conjecture for MZVs reads the same, but with $F_n$ replaced by $P_n$, the $n$th Padovan number (i.e., $P_0 = 1$, $P_1 = 0$, $P_2 = 1$, $P_n = P_{n-2} + P_{n-3}$).
The Padovan number $P_n$ is known to be an upper bound on the dimension of the rational vector space generated by the MZVs of weight $n$. If we denote by $\mathcal{MZV}_n$ and $\mathcal{MtV}_n$, respectively, the rational vector spaces generated by weight-$n$ MZVs and MtVs, we can judge their relative growth by comparing $P_n$ and $F_n$.

<table>
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<td>$F_n = \dim_{\mathbb{Q}} \mathcal{MtV}_n$?</td>
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<td>8</td>
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Evidently there are a lot more relations among MZVs than among MtVs.
MtVs as multiple Hurwitz zeta functions

Several results about multiple $t$-values are scattered about the literature, in a variety of different notations. Sometimes they are discussed in terms of multiple Hurwitz zeta values, defined by

$$
\zeta(a_1, \ldots, a_k; p_1, \ldots, p_k) = \sum_{n_1 > \cdots > n_k \geq 1} \frac{1}{(n_1 + p_1)^{a_1} \cdots (n_k + p_k)^{a_k}}.
$$

Evidently

$$
t(a_1, \ldots, a_k) = 2^{-a_1 - \cdots - a_k} \zeta(a_1, \ldots, a_k; -\frac{1}{2}, \ldots, -\frac{1}{2}).
$$
Consider the algebra $\mathbb{Q}[[x_1, x_2, \ldots]]$ of formal power series in a countable set of commuting generators $x_1, x_2, \ldots$. This has a graded subalgebra $\mathcal{B}$ consisting of those series of bounded degree (where each $x_i$ has degree 1). An element of $f \in \mathcal{B}$ is a quasi-symmetric function if

$$\text{coefficient of } x_{i_1}^{a_1} x_{i_2}^{a_2} \cdots x_{i_k}^{a_k} \text{ in } f = \text{coefficient of } x_1^{a_1} x_2^{a_2} \cdots x_k^{a_k} \text{ in } f$$

whenever $i_1 < i_2 < \cdots < i_k$. The set of such $f$ is a subalgebra $\text{QSym}$ of $\mathcal{B}$, called the quasi-symmetric functions.
Quasi-symmetric functions cont’d

As a vector space, QSym has the basis consisting of monomial quasi-symmetric functions $M(a_1,\ldots,a_k)$, where $(a_1,\ldots,a_k)$ is a composition (ordered sequence) of positive integers and

$$M(a_1,\ldots,a_k) = \sum_{i_1<\cdots<i_k} x^{a_1}_{i_1} \cdots x^{a_k}_{i_k}.$$ 

QSym has as a subalgebra the symmetric functions Sym; the symmetric functions have the vector space basis

$$m_{a_1,\ldots,a_k} = \sum_{i_1,\ldots,i_k \text{ distinct}} x^{a_1}_{i_1} \cdots x^{a_k}_{i_k}$$

indexed by partitions (unordered sequences) of positive integers. Note that, e.g.,

$$m_{2,2,1} = M(2,2,1) + M(2,1,2) + M(1,2,2).$$
In fact, QSym is a polynomial algebra on certain of the $M_I$. We order compositions lexicographically, i.e,

$$(1) < (1, 1) < (1, 2) < (1, 2, 1) < \cdots$$

and call a composition $I$ Lyndon if $I < K$ for any proper factorization $I = JK$: e.g., $(1, 3)$ is Lyndon but $(1, 1)$ and $(1, 2, 1)$ aren’t. Then QSym is the polynomial algebra on the $M_I$ with $I$ Lyndon (Malvenuto and Reutenauer, 1995). Note that the only Lyndon composition ending in 1 is $(1)$. Let $QSym^0$ be the subalgebra of QSym generated by $M_I$ for $I \neq (1)$ Lyndon, so that $QSym = QSym^0[M_{(1)}]$. 
Quasi-symmetric functions and MtVs

The following result is well-known (Hoffman 1997).

**Theorem**

There is a homomorphism $\zeta : \text{QSym}^0 \rightarrow \mathbb{R}$ sending 1 to 1 and $M(a_1, a_2, \ldots, a_k)$ to $\zeta(a_1, a_2, \ldots a_k)$ for $a_1 \geq 2$.

There is an exact analogue for MtVs.

**Theorem**

There is a homomorphism $\theta : \text{QSym}^0 \rightarrow \mathbb{R}$ sending 1 to 1 and $M(a_1, a_2, \ldots, a_k)$ to $t(a_1, a_2, \ldots, a_k)$ for $a_1 \geq 2$.

It follows that if any linear combination of $t$-values is the image of a symmetric function, then it is actually expressible as a rational polynomial in the depth 1 $t$-values, e.g.,

$t(2, 3) + t(3, 2) = t(2)t(3) - t(5)$.
MtVs of repeated arguments

In particular, any $t$-value of repeated arguments is a rational polynomial in the $t(i)$. If we write $\{k\}_n$ for $k$ repeated $n$ times, then we have the following.

**Theorem**

*For integer $k \geq 2$, let $Z_k(x)$ be the generating function*

$$Z_k(x) = 1 + \sum_{i=1}^{\infty} \zeta(\{k\}_i)x^{ik}.$$

*Then the corresponding generating function for multiple $t$-values is*

$$1 + \sum_{i=1}^{\infty} t(\{k\}_i)x^{ik} = \frac{Z_k(x)}{Z_k(x/2)}.$$
MtVs of repeated arguments cont’d

Now the generating functions $Z_k(x)$ were studied in some detail back in the 1990’s: see Broadhurst, Borwein and Bradley 1997. From their results and the preceding theorem we have, e.g.,

$$t(\{4\}_n) = \frac{\pi^{4n}}{2^{2n}(4n)!}, \quad t(\{6\}_n) = \frac{\pi^{6n}}{(8n)(6n-1)!},$$

$$t(\{10\}_n) = \frac{\pi^{10n}(L_{10n} + 1)}{(32n)(10n-1)!},$$

where in the last formula $L_n$ is the $n$th Lucas number, i.e., $L_0 = 2$, $L_1 = 1$ and $L_n = L_{n-1} + L_{n-2}$.
Another area where results on MtVs closely parallel those on MZVs is in sums of elements of purely even arguments. If for \( k \leq n \) we let \( T(2n, k) \) be the sum of all MtVs of even arguments having depth \( k \) and weight \( 2n \), then Zhao 2015 showed that

\[
T(2n, k) = \sum_{j=0}^{\left\lfloor \frac{k-1}{2} \right\rfloor} \frac{(-1)^j \pi^{2j} t(2n - 2j)}{2^{2k-2}(2j)!k} \binom{2k - 2j - 2}{k - 1},
\]

following my result

\[
E(2n, k) = \sum_{j=0}^{\left\lfloor \frac{k-1}{2} \right\rfloor} \frac{(-1)^j \pi^{2j} \zeta(2n - 2j)}{2^{2n-2j-2}(2j + 1)!} \binom{2k - 2j - 1}{k},
\]

for \( E(2n, k) \) the sum of all MZVs of even arguments having depth \( k \) and weight \( 2n \).
Both formulas are proved from corresponding generating functions: we have the parallel results

$$\mathcal{T}(t, s) = 1 + \sum_{n=1}^{\infty} \sum_{k=1}^{n} T(2n, k) t^n s^k = \frac{\cos \left( \frac{\pi}{2} \sqrt{(1 - s)t} \right)}{\cos \left( \frac{\pi}{2} \sqrt{t} \right)}$$

and

$$\mathcal{E}(t, s) = 1 + \sum_{n=1}^{\infty} \sum_{k=1}^{n} E(2n, k) t^n s^k = \frac{\sin \left( \pi \sqrt{1 - s} \right)}{\sqrt{1 - s} \sin(\pi \sqrt{t})}.$$

These in turn follow from taking images under appropriate homomorphisms of the generating function.
Generating functions cont’d

\[ \mathcal{F}(t, s) = 1 + \sum_{n=1}^{\infty} \sum_{k=1}^{n} N_{n,k} t^n s^k \in \text{QSym}[[t, s]], \]

where \( N_{n,k} \) is the sum of all monomial symmetric functions corresponding of partitions of \( n \) with \( k \) parts. In fact

\[ \mathcal{E}(t, s) = \zeta \mathcal{P}_2 \mathcal{F}(t, s) \quad \text{and} \quad \mathcal{I}(t, s) = \theta \mathcal{P}_2 \mathcal{F}(t, s) \]

where \( \mathcal{P}_2 : \text{QSym} \to \text{QSym} \) sends each \( x_i \) to \( x_i^2 \). The formulas on the preceding slide then follow from

\[ \mathcal{F}(t, s) = H(t) E((s - 1)t), \]

where \( H(t) \) and \( E(t) \) are respectively the generating functions for the complete and elementary symmetric functions.
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Iterated integral representations

Call a sequence of \((a_1, \ldots, a_k)\) of positive integers admissible if \(a_1 > 1\). Now if

\[
\omega_0 = \frac{dt}{t}, \quad \omega_1 = \frac{dt}{1-t}, \quad \omega_{-1} = \frac{dt}{1+t},
\]

then there is the well-known representation of MZVs

\[
\zeta(a_1, \ldots, a_k) = \int_0^1 \omega_0^{a_1-1} \omega_1 \cdots \omega_0^{a_k-1} \omega_1
\]

for any admissible sequence \((a_1, \ldots, a_k)\). This can be extended as follows. Let \(P\) be the set of positive integers, \(\tilde{P} = \{\ldots, 3, 2, 1, 2, 3, \ldots\}\). The set \(\{-1, 1\}\) acts on \(\tilde{P}\) as follows: \(1 \circ n = n, \ 1 \circ \bar{n} = \bar{n},\ (-1) \circ n = \bar{n}, \ (-1) \circ \bar{n} = n\). For \(a \in \tilde{P}\), let \(\text{sgn}(a) = 1\) if \(a \in P\) and \(-1\) otherwise. Note \(\text{sgn}(a) \circ a \in P\).
Alternating MZVs

For $b_1, \ldots, b_k \in \tilde{P}$ with $b_1 \neq 1$, define the alternating MZV by

$$\zeta(b_1, \ldots, b_k) = \sum_{n_1 \gg \cdots > n_k \geq 1} \frac{\text{sgn}(b_1)^{n_1} \cdots \text{sgn}(b_k)^{n_k}}{n_1 \text{sgn}(b_1) \circ b_1 \cdots n_k \text{sgn}(b_k) \circ b_k}.$$ 

Now let $(a_1, \ldots, a_k)$ be admissible. If $\epsilon_1, \ldots, \epsilon_k \in \{-1, 1\}$, then

$$\int_0^1 \omega_0^{a_1-1} \omega_{\epsilon_1} \cdots \omega_0^{a_k-1} \omega_{\epsilon_k} =$$

$$\epsilon_1 \cdots \epsilon_k \zeta(\epsilon_1 \circ a_1, \epsilon_1 \epsilon_2 \circ a_2, \epsilon_2 \epsilon_3 \circ a_3, \ldots, \epsilon_{k-1} \epsilon_k \circ a_k)$$
For multiple $t$-values there is also an iterated integral representation, but it is not so simple.

**Proposition**

For any admissible sequence $(a_1, \ldots, a_k)$,

$$t(a_1, \ldots, a_k) = \int_0^1 \omega_0^{a_1-1} \Omega_a \cdots \omega_0^{a_k-1} \Omega_a \omega_0^{a_k-1} \Omega_b$$

where

$$\Omega_a = \frac{tdt}{1 - t^2} = \frac{1}{2}(\omega_1 - \omega_{-1}), \quad \Omega_b = \frac{dt}{1 - t^2} = \frac{1}{2}(\omega_1 + \omega_{-1}).$$
MtVs and alternating MZVs

Expanding out the preceding result and using the extended integral representation of alternating MZVs gives the following.

**Theorem**

For an admissible sequence \((a_1, \ldots, a_k)\), the multiple t-value \(t(a_1, \ldots, a_k)\) is given by

\[
\frac{1}{2^k} \sum_{\epsilon_1, \ldots, \epsilon_k} \epsilon_1 \cdots \epsilon_k \zeta(\epsilon_1 \circ a_1, \ldots, \epsilon_k \circ a_k),
\]

where the sum is over the \(2^k\) \(k\)-tuples \((\epsilon_1, \ldots, \epsilon_k)\) with \(\epsilon_i \in \{-1, 1\}\).

This expresses \(t(a_1, \ldots, a_k)\) as a sum of \(2^k\) alternating MZVs.
But it’s possible to do better. For admissible \((a_1, \ldots, a_k)\) and \(p \leq k\), let \(L_p \zeta(a_1, \ldots, a_k)\) be the sum of the \(\binom{k}{p}\) alternating MZVs in which \((-1)^{\circ}\) is applied to exactly \(p\) of the arguments.

**Theorem**

*For an admissible sequence \((a_1, \ldots, a_k)\), the multiple t-value \(t(a_1, \ldots, a_k)\) is given by*

\[
\frac{1}{2a_1+\ldots+a_k} \zeta(a_1, \ldots, a_k) - \frac{1}{2^{k-1}} \sum_{p \leq k \text{ odd}} L_p \zeta(a_1, \ldots, a_k).
\]

This expresses \(t(a_1, \ldots, a_k)\) as a sum of \(2^{k-1} + 1\) alternating MZVs.
MtVs and alternating MZVs cont’d

Even for double $t$-values this is an improvement; it replaces

$$t(a, b) = \frac{1}{4} \left[ \zeta(a, b) - \zeta(a, \bar{b}) - \zeta(\bar{a}, b) + \zeta(\bar{a}, \bar{b}) \right]$$

with

$$t(a, b) = \frac{1}{2^{a+b}} \zeta(a, b) - \frac{1}{2} \left[ \zeta(a, \bar{b}) + \zeta(\bar{a}, b) \right].$$

For triple $t$-values we have

$$t(a, b, c) = \frac{1}{2^{a+b+c}} \zeta(a, b, c)$$

$$- \frac{1}{4} \left[ \zeta(a, b, \bar{c}) + \zeta(a, \bar{b}, c) + \zeta(\bar{a}, b, c) + \zeta(\bar{a}, \bar{b}, \bar{c}) \right].$$
Using the preceding result, we can expand any MtV into a sum of alternating MZVs. For example,

\[
t(2, 3, 1) = \frac{1}{64} \zeta(2, 3, 1) - \frac{1}{4} \left[ \zeta(\bar{2}, 3, 1) + \zeta(2, \bar{3}, 1) + \zeta(2, 3, \bar{1}) + \zeta(\bar{2}, \bar{3}, \bar{1}) \right].
\]

Now we can use tables from the Multiple Zeta Value Data Mine project of Blümlein, Broadhurst and Vermaseren to expand each of the alternating MZVs in this sum, resulting in

\[
t(2, 3, 1) = -\frac{2}{21} t(6) - \frac{3}{196} t(3)^2 - \frac{1}{2} t(2) \zeta(\bar{3}, 1) + \frac{1}{4} \zeta(\bar{5}, 1)
- \frac{1}{2} t(5) \log 2 + \frac{4}{7} t(2) t(3) \log 2.
\]
Similarly we have obtained formulas for all multiple $t$-values of weight $\leq 7$. In our tables we have

$$t(2, 3) = -\frac{1}{2}t(5) + \frac{4}{7}t(2)t(3).$$

This and many similar instances have led us to the following conjecture.

**Conjecture**

*Every multiple* $t$*-value admits a representation as a polynomial in the* $t(i)$, $i \geq 2$, log $2$, and selected alternating MZVs *in such a way that*

$$\frac{\partial t(s, 1)}{\partial \log 2} = t(s).$$

*for any admissible sequence* $s$. 
Consider the function $A_- : \text{QSym} \to \text{QSym}$ given by

$$A_- (M_{(i_1, \ldots, i_k)}) = \begin{cases} M_{(i_1, \ldots, i_{k-1})}, & \text{if } i_k = 1, \\ 0, & \text{otherwise.} \end{cases}$$

Then $A_-$ is a derivation of QSym, and it restricts to a derivation of QSym$^0$. The conjecture above can be restated as follows.

**Conjecture**

*There is a derivation $d$ on $\mathbb{M}t\mathcal{V} = \theta(\text{QSym}^0)$ such that $\theta A_- = d\theta$.*

Note that if there were a derivation $\partial$ on $\mathbb{M}\mathcal{Z}\mathcal{V} = \zeta(\text{QSym}^0)$ such that $\zeta A_- = \partial \zeta$, then we’d have the contradiction

$$0 = \zeta(A_- M_3) = \partial \zeta(3) = \partial \zeta(2, 1) = \zeta(A_- M_{(2,1)}) = \zeta(2).$$
The second conjecture, which we have already mentioned, is based on computations of the rank of the set of multiple \( t \)-values of a given weight. Based on our tables through weight 7, we have computed the ranks (starting in weight 2) as

\[ 1, 2, 3, 5, 8, 13 \]

which leads to the following “Fibonacci Conjecture.”

**Conjecture**

*If \( \mathcal{MtV}_n \) is the rational vector subspace of \( \mathbb{R} \) spanned by weight-\( n \) multiple \( t \)-values, then \( \dim_{\mathbb{Q}} \mathcal{MtV}_n = F_n \), the \( n \)th Fibonacci number.*
Of course the existing evidence for the Fibonacci Conjecture is rather thin. The Multiple Zeta Value Data Mine actually has publically available files on altering MZVs for weights through 14, so there is plenty of testing yet to do even without extending their work. But this gets laborious: in weight 7 there are 32 admissible sequences, and the sum for $t(2,1,1,1,1,1)$ has 33 terms. Blümlein, Broadhurst and Vermaseren are all particle physicists, with plenty of experience with large-scale calculations, so they probably have helpful ideas on how to manage the higher weights.
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One place where the theories of MZVs and MtVs are closely parallel is in depth 2. It is convenient to define

$$N(a, b, i) = \binom{2i - 2}{a - 1} + \binom{2i - 2}{b - 1},$$

where $\binom{p}{j} = 0$ if $j > p$. It is well-known (and implicit in Euler’s 1776 paper) that

$$\zeta(a, b) = \frac{(-1)^a}{2} \left( \binom{a + b}{a} - 1 \right) \zeta(2n + 1) +$$

$$\begin{cases} 
\zeta(a)\zeta(b) - \sum_{i=2}^{n} N(a, b, i)\zeta(2i - 1)\zeta(2n - 2i + 2), & a \text{ even}, \\
\sum_{i=2}^{n} N(a, b, i)\zeta(2i - 1)\zeta(2n - 2i + 2), & \text{otherwise}.
\end{cases}$$

if $a + b = 2n + 1$ and $a, b \geq 2$ (No general formula in terms of single zeta values is known for $\zeta(a, b)$ if $a + b$ is even.)
For $\zeta(2n, 1)$ one has another formula

$$
\zeta(2n, 1) = n\zeta(2n + 1) - \frac{1}{2} \sum_{i=2}^{2n-1} \zeta(i)\zeta(2n + 1 - i).
$$

Basu 2008 gave the similar formula

$$
t(a, b) = -\frac{1}{2} t(2n + 1) + \\
\begin{cases}
  t(a)t(b) - \sum_{i=2}^{n} N(a, b, i) \frac{t(2i-2)t(2n-2i+2)}{2^{2i-1}-1}, & a \text{ even,} \\
  \sum_{i=2}^{n} N(a, b, i) \frac{t(2i-1)t(2n-2i+2)}{2^{2i-1}-1}, & \text{otherwise,}
\end{cases}
$$

for $a + b = 2n + 1$. Basu actually stipulates that $a, b \geq 2$, but if we take $a = 2n$, $b = 1$ and set $t(1) = \log 2$ the formula is still valid (as follows from Jordan 1973 or Nakamura and Tasaka 2013).
Explicit formulas in depth 2 cont’d

The proofs used by Basu and Nakamura-Tasaka are elementary but different. I have been able to prove the $a = 2n$, $b = 1$ case, that is,

\[ t(2n, 1) = -\frac{1}{2} t(2n + 1) + t(2n) \log 2 \]

\[ - \sum_{i=2}^{n} \frac{t(2i - 1)t(2n - 2i + 2)}{2^{2i-1} - 1}, \]

using yet another elementary method. I believe this can be extended to the general case $a + b = 2n + 1$, though I haven’t yet done this. My method involves modified Tornheim sums.
Tornheim sums

The depth 2 formulas for the MZV case can all be rather neatly proved using sums invented in Tornheim 1950:

\[ T(a, b, c) = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{1}{i^a j^b (i + j)^c}. \]

They have the properties \( T(a, b, c) = T(b, a, c), \)
\( T(a, 0, c) = \zeta(c, a) \) for \( c > 1, \)
\( T(a, b, 0) = \zeta(a) \zeta(b) \) for \( a, b \geq 2, \) and

\[ T(a, b, c) = T(a - 1, b, c + 1) + T(a, b - 1, c + 1) \]

for \( a, b \geq 1. \)
Modified Tornheim sums

For the $t$-values one can use a modified Tornheim sum

$$M(a, b, c) = \sum_{i=1}^{\infty} \sum_{j=0}^{\infty} \frac{1}{(2i)^a(2j+1)^b(2i+2j+1)^c}$$

One has $M(0, b, c) = t(c, b)$ for $c > 1$, $M(a, b, 0) = 2^{-a}\zeta(a)t(b)$ for $a, b \geq 2$ and

$$M(a, b, c) = M(a - 1, b, c + 1) + M(a, b - 1, c + 1)$$

for $a, b \geq 1$, but the symmetry in the first two arguments is lost and $M(a, 0, c)$ is not particularly simple. Nevertheless, one can mimic many of the arguments used for Tornheim sums.
Here is an interesting point of difference between $T$ and $M$. By partial fractions one has

$$T(1, p, 1) = \sum_{j=1}^{\infty} \frac{1}{jp+1} \sum_{i=1}^{\infty} \left[ \frac{1}{i} - \frac{1}{i+j} \right],$$

and the inner sum telescopes to give

$$\sum_{j=1}^{\infty} \frac{1}{jp+1} \left[ 1 + \cdots + \frac{1}{j} \right] = \zeta(p+2) + \zeta(p+1, 1).$$
But in the corresponding sum

$$M(1, p, 1) = \sum_{j=0}^{\infty} \frac{1}{(2j+1)^{p+1}} \sum_{i=1}^{\infty} \left[ \frac{1}{2i} - \frac{1}{2i + 2j + 1} \right]$$

the inner sum does not telescope, and instead we have

$$\sum_{j=0}^{\infty} \frac{1}{(2j+1)^{p+1}} \left[ -\log 2 + 1 + \frac{1}{3} + \cdots + \frac{1}{2j+1} \right]$$

$$= t(p + 2) + t(p + 1, 1) - t(p + 1) \log 2.$$
A formula for $t(2n + 1, 1)$

The argument for $t(2n, 1)$ can be modified slightly to give a formula for $t(2n + 1, 1)$ (but one must pay the price of including an alternating MZV):

$$
t(2n + 1, 1) = t(2n + 1) \log 2 - \frac{1}{2} \zeta(2n + 1, 1) + \frac{(2n + 1)(1 - 2^{2n+1}) - 2^{2n+2}}{4(2^{2n+2} - 1)} t(2n + 2) +$$

$$\sum_{i=1}^{n-1} \frac{2^{2n+1} - 2^{2i+1} - 2^{2n-2i+1} + 1}{2(2^{2i+1} - 1)(2^{2n-2i+1} - 1)} t(2i + 1) t(2n - 2i + 1).$$