Standard Relations of Multiple Polylogarithm Values at Roots of Unity

Dedicated to Prof. Keqin Feng on his 70th birthday

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Abstract. Let N be a positive integer. In this paper we shall study the special values of multiple polylogarithms at Nth roots of unity, called multiple polylogarithm values (MPVs) of level N. Our primary goal in this paper is to investigate the relations among the MPVs of the same weight and level by using the regularized double shuffle relations, regularized distribution relations, lifted versions of such relations from lower weights, and weight one relations which are produced by relations of weight one MPVs. We call relations from the above four families *standard*. Let $d(w,N)$ be the dimension of the $\mathbb{Q}$-vector space generated by all MPVs of weight w and level N. Recently Deligne and Goncharov were able to obtain some lower bound of $d(w,N)$ using the motivic mechanism. We call a level N *standard* if $N=1,2,3$ or $N=p^n$ for prime $p\ge 5$. Our computation suggests the following dichotomy: If N is standard then the standard relations should produce all the linear relations and if further $N>3$ then the bound of $d(w,N)$ by Deligne and Goncharov can be improved; otherwise there should be non-standard relations among MPVs for all sufficiently large weights (depending only on N) and the bound by Deligne and Goncharov may be sharp. We write down some of the non-standard relations explicitly with good numerical verification. In two instances ($N=4$, $w=3,4$) we can rigorously prove these relations by using the octahedral symmetry of $\{0,\infty,\pm1,\pm\sqrt{-1}\}$. Throughout the paper we provide many conjectures which are strongly supported by computational evidence.

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Contents

1 Introduction

In recent years, there is a revival of interest in multi-valued classical polylogarithms (polylogs) and their generalizations. For any positive integers $s_1,\dots,s_\ell$, multiple polylogs of complex variables are defined as follows (note that our index order is opposite to that of [19]):

$$Li_{s_1,\dots,s_\ell}(x_1,\dots,x_\ell)=\sum_{k_1>\cdots>k_\ell>0}\frac{x_1^{k_1}\cdots x_\ell^{k_\ell}}{k_1^{s_1}\cdots k_\ell^{s_\ell}}, \tag{1}$$

where $|x_1\cdots x_j|<1$ for $j=1,\dots,\ell$. It can be analytically continued to a multi-valued meromorhpic function on $\mathbb{C}^\ell$ (see [29]). Conventionally ℓ is called the *depth* (or *length*) and $s_1 + \cdots + s_\ell$ the *weight*. When the depth $\ell = 1$ the function is nothing but the classical polylog. When the weight is also 1 one gets the MacLaurin series of $-\log(1-x)$. Moreover, setting $x_1 = \cdots = x_\ell = 1$ and $s_1 > 1$ one obtains the well-known multiple zeta values (MZVs). If one allows x_j's to be ± 1 then one gets the so-called alternating Euler sums.

1.1 Multiple polylog values at roots of unity

In this paper, the primary objects of study are the multiple polylog values at roots of unity (MPVs). These special values, MZVs and the alternating Euler sums in particular, have attracted a lot attention in recent years after they were found to be connected to many branches of mathematics and physics (see, for e.g., [7, 8, 10, 11, 15, 19, 28]). Results up to around year 2000 can be found in the comprehensive survey paper [6].
Starting from early 1990s Hoffman [21, 22] has constructed some quasi-shuffle (called *stuffle* in [6]) algebras reflecting the essential combinatorial properties of MZVs. Later he [23] extends this to incorporate MPVs although his definition of $*$-product is different from ours. This approach was then improved in [24] and [26] to study MZVs and MPVs in general, respectively, where the regularized double shuffle relations play prominent roles. One derives these relations by comparing (1) with another expression of the multiple polylogs given by the following iterated integral:

$$Li_{s_1,\dots,s_\ell}(x_1,\dots,x_\ell) = (-1)^\ell \int_0^1 \left(\frac{dt}{t}\right)^{\circ(s_1-1)} \circ \frac{dt}{t-a_1} \circ \cdots \circ \left(\frac{dt}{t}\right)^{\circ(s_\ell-1)} \circ \frac{dt}{t-a_\ell}, \quad (2)$$

where $a_i = 1/(x_1 \dots x_i)$ for $1 \le i \le \ell$. Here, one defines the iterated integrals recursively by $\int_a^b f(t) \circ w(t) = \int_a^b (\int_a^x w(t)) f(x)$ for any 1-form $w(t)$ and concatenation of 1-forms $f(t)$. One may think the path lies in $\mathbb{C}$; however, it is more revealing to use iterated integrals in $\mathbb{C}^\ell$ to find the analytic continuation of this function (see [29]).
The main feature of this paper is a quantitative comparison between the results obtained by Racinet [26] who considers MPVs from the motivic viewpoint of Drinfeld associators, and those by Deligne and Goncharov [17] who study the motivic fundamental groups of $\mathbb{P}^1 - (\{0,\infty\} \cup \boldsymbol{\mu}_N)$ by using the theory of mixed Tate motives over S-integers of number fields, where $\boldsymbol{\mu}_N$ is the group of Nth roots of unity.
Fix an Nth root of unity $\mu = \mu_N := \exp(2\pi\sqrt{-1}/N)$. An MPV of *level* N is a number of the form

$$L_N(s_1,\dots,s_\ell | i_1,\dots,i_\ell) := Li_{s_1,\dots,s_\ell}(\mu^{i_1},\dots,\mu^{i_\ell}). \quad (3)$$

We will always identify $(i_1,\dots,i_\ell)$ with $(i_1,\dots,i_\ell) \pmod N$. It is easy to see from (1) that an MPV converges if and only if $(s_1, \mu^{i_1}) \ne (1,1)$. Clearly, all

MPVs of level N are automatically of level Nk for every positive integer k. For example when $i_1 = \cdots = i_\ell = 0$ or $N = 1$ one gets the MZV $\zeta(s_1, \dots, s_\ell)$. When $N = 2$ one recovers the alternating Euler sums studied in [8, 31]. To save space, if a string S repeats n times then $\{S\}^n$ will be used. For example, $L_N(\{2\}^2|\{0\}^2) = \zeta(2,2) = \pi^4/120$.

Standard conjectures in arithmetic geometry imply that $\mathbb{Q}$-linear relations among MVPs can only exist between those of the same weight. Let $\mathcal{MPV}(w,N)$ be the $\mathbb{Q}$-span of all the MPVs of weight w and level N. Let $d(w,N)$ denoted its dimension. In general, it is very difficult to determine $d(w,N)$ because any nontrivial lower bound would provide some nontrivial irrational/transcendental result which is related to a variant of Grothendieck's period conjecture (see [16] or [17, 5.27(c)]). For example, one can show easily that $\mathcal{MPV}(2,4) = \langle \log^2 2, \pi^2, \pi \log 2\sqrt{-1}, (K-1)\sqrt{-1}\rangle$, where $K = \sum_{n\ge 0}(-1)^n/(2n+1)^2$ is the Catalan's constant. From a variant of Grothendieck's period conjecture we know $d(2,4) = 4$ (see [16]) but we don't have an unconditional proof yet. Namely, we cannot prove that the four number $\log^2 2, \pi^2, \pi \log 2\sqrt{-1}, (K-1)\sqrt{-1}$ are linearly independent over $\mathbb{Q}$. Thus, nontrivial lower bound of $d(w,N)$ is hard to come by.

On the other hand, one may obtain upper bound of $d(w,N)$ by finding as many linear relations in $\mathcal{MPV}(w,N)$ as possible. As in the cases of MZVs and the alternating Euler sums the double shuffle relations play important roles in revealing the relations among MPVs. In such a relation if all the MPVs involved are convergent it is called a *finite double shuffle relation* (FDS). In general one needs to use regularization to obtain *regularized double shuffle* relations (RDS) involving divergent MPVs. We shall recall this theory in §2 building on the results of [24, 26].

From the point of view of Lyndon words and quasi-symmetric functions Bigotte et al. [3, 4] have studied MPVs (they call them *colored MZVs*) primarily by using double shuffle relations and monodromy argument (cf. [4, Thm. 5.1]). However, when the level $N \ge 2$, these double shuffle relations often are not complete, as we shall see in this paper (for level two, see also [5]).

1.2 Standard relations of MPVs

If the level $N > 3$ then there are many non-trivial linear relations in $\mathcal{MPV}(1,N)$ of weight one whose structure is clear to us. Multiplied by MPVs of weight $w-1$ these relations can produce non-trivial linear relations among MPVs of weight w which are called the *weight one relations.* Similar to these relations one may produce new relations by multiplying MPVs on all of the other types of relations among MPVs of lower weights. We call such relations *lifted relations.*

It is well-known that among MPVs there are the so-called *finite distribution relations* (FDT), see (14). Racinet [26] further considers the regularization of these relations by regarding MPVs as the coefficients of some group-like element in a suitably defined pro-Lie-algebra of motivic origin (see §4). Our computation shows that the *regularized distribution relations* (RDT) do contribute to new relations not covered by RDS and FDT. But they are not enough yet to produce all the lifted RDS.

Definition 1.1. We call a $\mathbb{Q}$-linear relation between MPVs *standard*[1] if it can be produced by some $\mathbb{Q}$-linear combinations of the following four families of relations: regularized double shuffle relations (RDS), regularized distribution relations (RDT), weight one relations, and lifted relations from the above. Otherwise, it is called a *non-standard* relation.

It is commonly believed that all linear relations among MPVs (i.e. levels one MPVs) are consequences of RDS. When level $N = 2$ we believe that all linear relations among the alternating Euler sums are consequences of RDS and RDT. Further, in this case, the RDT should correspond to the doubling and generalized doubling relations of [5].

1.3 Main results

The main goal of this paper is to provide some extensive numerical evidence concerning the (in)completeness of the standard relations. Namely, these relations in general are not enough to produce all the $\mathbb{Q}$-linear relation between MPVs (see Remark 8.2 and Conjecture 8.5); however, we have the following result (see Thm. 8.6 and Thm. 8.3).

Theorem 1.2. *Let $p \ge 5$ be a prime. Then $d(2,p) \le (5p+7)(p+1)/24$ and $d(2,p^2) < (p^2-p+2)^2/4$. If a variant of Grothendieck's period conjecture* [17, 5.27(c)] *is true then the equality holds for $d(2,p)$ and the standard relations in $\mathcal{MPV}(2,p)$ imply all the others.*

If weight $w = 2$ and $N = 5^2, 7^2, 11^2, 13^2$ or 5^3, then our computation (see Table 1) shows that the standard relations are very likely to be complete. However, if $N > 3$ is a 2-power or 3-power or has at least two distinct prime factors then the standard relations are often incomplete. Moreover, we don't know how to obtain the non-standard relations rigorously except that when the level $N = 4$ we get (see Thm. 9.1)

Theorem 1.3. *If the conjecture in* [17, 5.27(c)] *is true then all the linear relations among MPVs of level four and weight three (resp. weight four) are the consequences of the standard relations and the octahedral relation* (53) *(resp. the five octahedral relations* (54)-(58)*).*

Most of the MPV identities in this paper are discovered with the help of MAPLE using symbolic computations. We have verified all relations numerically by GiNaC [27] with an error bound $< 10^{-90}$. Some results contained in this paper were announced in [30].

[1] This term was suggested by P. Deligne in a letter to Goncharov and Racinet dated Feb. 25, 2008.

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2 The double shuffle relations and the algebra $\mathfrak{A}$

In this section we recall the procedure to transform the shuffle relations among MPVs into some pure algebra structures. This is a rather straight-forward variation of a theme first studied by Hoffman for MZVs (see, for e.g., [22, 23]) and then further developed by Ihara et al. in [24] and by Racinet in [26]. Most of the results in this section are well-known but we include them for the convenience of the reader.

It is Kontsevich [25] who first noticed that MZVs can be represented by iterated integrals. One can easily extend this to MPVs [26]. Set

$$a = \frac{dt}{t}, \qquad b_i = \frac{\mu^i dt}{1-\mu^i t} \quad \text{for } i = 0, 1, \dots, N-1.$$

For every positive integer n define the word of length n

$$y_{n,i} := a^{n-1} b_i.$$

Then it is straight-forward to verify using (2) that if $(s_1, \mu^{i_1}) \neq (1,1)$ then (cf. [26, (2.5)])

$$L_N(s_1, \dots, s_n | i_1, i_2, \dots, i_n) = \int_0^1 y_{s_1,i_1} y_{s_2,i_1+i_2} \cdots y_{s_n,i_1+i_2+\cdots+i_n}. \qquad (4)$$

One can now define an algebra of words as follows:

Definition 2.1. Set $A_0 = \{\mathbf{1}\}$ to be the set of the empty word. Define $\mathfrak{A} = \mathbb{Q}\langle A\rangle$ to be the graded noncommutative polynomial $\mathbb{Q}$-algebra generated by letters a and b_i for $i \equiv 0, \dots, N-1 \pmod N$, where A is a locally finite set of generators whose degree n part A_n consists of words (i.e., a monomial in the letters) of depth n. Let $\mathfrak{A}^0$ be the subalgebra of $\mathfrak{A}$ generated by words not beginning with b_0 and not ending with a. The words in $\mathfrak{A}^0$ are called *admissible words.*

Observe that every MPV can be expressed as an iterated integral over the closed interval $[0,1]$ of an admissible word w in $\mathfrak{A}^0$. This is denoted by

$$Z(w) := \int_0^1 w. \tag{5}$$

We remark that the length $\lg(w)$ of w is equal to the weight of $Z(w)$. Therefore in general one has (cf. [26, (2.5) and (2.6)])

$$L_N(s_1,\dots,s_n|i_1,i_2,\dots,i_n) = Z(y_{s_1,i_1}y_{s_2,i_1+i_2}\cdots y_{s_n,i_1+i_2+\cdots+i_n}), \tag{6}$$
$$Z(y_{s_1,i_1}y_{s_2,i_2}\cdots y_{s_n,i_n}) = L_N(s_1,\dots,s_n|i_1,i_2-i_1,\dots,i_n-i_{n-1}). \tag{7}$$

For example $L_3(1,2,2|1,0,2) = Z(y_{1,1}y_{2,1}y_{2,0})$. On the other hand, during 1960s Chen developed a theory of iterated integral which can be applied in our situation.

Lemma 2.2. ([12, (1.5.1)]) *Let ω_i $(i \ge 1)$ be $\mathbb{C}$-valued 1-forms on a manifold M. For every path p,*

$$\int_p \omega_1\cdots\omega_r \int_p \omega_{r+1}\cdots\omega_{r+s} = \int_p (\omega_1\cdots\omega_r)ш(\omega_{r+1}\cdots\omega_{r+s})$$

where ш is the shuffle product defined by

$$(\omega_1\cdots\omega_r)ш(\omega_{r+1}\cdots\omega_{r+s}) := \sum_{\substack{\sigma\in S_{r+s},\sigma^{-1}(1)<\cdots<\sigma^{-1}(r)\\ \sigma^{-1}(r+1)<\cdots<\sigma^{-1}(r+s)}} \omega_{\sigma(1)}\cdots\omega_{\sigma(r+s)}.$$

For example, one has

$$\begin{aligned} & L_N(1|1)L_N(2,3|1,2) = Z(y_{1,1})Z(y_{2,1}y_{3,3}) = Z(b_1ш(ab_1a^2b_3)) \\ =& Z(b_1ab_1a^2b_3 + 2ab_1^2a^2b_3 + (ab_1)^2ab_3 + ab_1a^2b_1b_3 + ab_1a^2b_3b_1) \\ =& Z(y_{1,1}y_{2,1}y_{3,3} + 2y_{2,1}y_{1,1}y_{3,3} + y_{2,1}^2y_{2,3} + y_{2,1}y_{3,1}y_{1,3} + y_{2,1}y_{3,3}y_{1,1}) \\ =& L_N(1,2,3|1,0,2) + 2L_N(2,1,3|1,0,2) + L_N(2,2,2|1,0,2) \\ & \qquad + L_N(2,3,1|1,0,2) + L_N(2,3,1|1,2,N-2). \end{aligned}$$

Let $\mathfrak{A}_ш$ be the algebra of $\mathfrak{A}$ together with the multiplication defined by shuffle product ш. Denote the subalgebra $\mathfrak{A}^0$ by $\mathfrak{A}^0_ш$ when one considers the shuffle product. Then one can easily prove

Proposition 2.3. *The map $Z : \mathfrak{A}^0_ш \longrightarrow \mathbb{C}$ is an algebra homomorphism.*

On the other hand, MPVs are known to satisfy the series stuffle relations. For example

$$L_N(2|5)L_N(3|4) = L_N(2,3|5,4) + L_N(3,2|4,5) + L_N(5|9).$$

To study such relations in general one has the following definition.

Definition 2.4. Denote by $\mathfrak{A}^1$ the subalgebra of $\mathfrak{A}$ which is generated by words $y_{s,i}$ with $s \in \mathbb{N}$ and $i \equiv 0, \dots, N-1 \pmod{N}$. Equivalently, $\mathfrak{A}^1$ is the subalgebra of $\mathfrak{A}$ generated by words not ending with a. For any word $w = y_{s_1,i_1} y_{s_2,i_2} \cdots y_{s_n,i_n} \in \mathfrak{A}^1$ and positive integer j one defines the exponent shifting operator τ_j by

$$\tau_j(w) = y_{s_1,j+i_1} y_{s_2,j+i_2} \cdots y_{s_n,j+i_n}.$$

For convenience, on the empty word we adopt the convention that $\tau_j(\mathbf{1}) = \mathbf{1}$. We then define another multiplication $*$ on $\mathfrak{A}^1$ by requiring that $*$ distribute over addition, that $\mathbf{1} * w = w * \mathbf{1} = w$ for any word w, and that, for any words ω_1, ω_2,

$$y_{s,j}\omega_1 * y_{t,k}\omega_2 = y_{s,j}\Big(\tau_j\big(\tau_{-j}(\omega_1) * y_{t,k}\omega_2\big)\Big) + y_{t,k}\Big(\tau_k\big(y_{s,j}\omega_1 * \tau_{-k}(\omega_2)\big)\Big) + y_{s+t,j+k}\Big(\tau_{j+k}\big(\tau_{-j}(\omega_1) * \tau_{-k}(\omega_2)\big)\Big). \quad (8)$$

This multiplication is called the *stuffle product* in [6].

If one denotes by $\mathfrak{A}^1_*$ the algebra $(\mathfrak{A}^1, *)$ then it is not hard to show that

Proposition 2.5. (cf. [22, Thm. 2.1]) *The polynomial algebra $\mathfrak{A}^1_*$ is a commutative graded $\mathbb{Q}$-algebra.*

Now one can define the subalgebra $\mathfrak{A}^0_*$ similar to $\mathfrak{A}^0_{ш}$ by replacing the shuffle product by the stuffle product. Then by induction on the lengths and using the series definition one can quickly check that for any $\omega_1, \omega_2 \in \mathfrak{A}^0_*$

$$Z(\omega_1)Z(\omega_2) = Z(\omega_1 * \omega_2).$$

This implies that

Proposition 2.6. *The map $Z : \mathfrak{A}^0_* \longrightarrow \mathbb{C}$ is an algebra homomorphism.*

Definition 2.7. Let w be a positive integer such that $w \geq 2$. For nontrivial $\omega_1, \omega_2 \in \mathfrak{A}^0$ with $\lg(\omega_1) + \lg(\omega_2) = w$ one says that

$$Z(\omega_1 ш \omega_2 - \omega_1 * \omega_2) = 0 \quad (9)$$

is a *finite double shuffle* relation (FDS) of weight w.

It is known that even in level one these relations are not enough to provide all the relations among MZVs. However, it is believed that one can remedy this by considering *regularized double shuffle* relation (RDS) produced by the following mechanism. This is explained in detail in [24] when Ihara, Kaneko and Zagier consider MZVs where they call these *extended double shuffle* relations or EDS. It is also contained in [26] with a different formulation.
To produce RDS, first, combining Propositions 2.6 and 2.3 one can easily prove the following algebraic result (cf. [24, Prop. 1]):

Proposition 2.8. *One has two algebra homomorphisms:*

$$Z^* : (\mathfrak{A}^1_*, *) \longrightarrow \mathbb{C}[T], \quad \text{and} \quad Z^ш : (\mathfrak{A}^1_ш, ш) \longrightarrow \mathbb{C}[T]$$

which are uniquely determined by the properties that they both extend the evaluation map $Z : \mathfrak{A}^0 \longrightarrow \mathbb{C}$ by sending $b_0 = y_{1,0}$ to T.

Second, in order to establish the crucial relation between Z^* and $Z^ш$ one can adopt the machinery in [24] as follows. For any $(\mathbf{s}|\mathbf{i}) = (s_1, \ldots, s_n | i_1, \ldots, i_n)$ where i_j's are integers and s_j's are positive integers, let the image of the corresponding words in $\mathfrak{A}^1$ under Z^* and $Z^ш$ be denoted by $Z^*_{(\mathbf{s}|\mathbf{i})}(T)$ and $Z^ш_{(\mathbf{s}|\mathbf{i})}(T)$ respectively.

Theorem 2.9. (cf. [26, Cor. 2.24]) *Define a $\mathbb{C}$-linear map $\rho : \mathbb{C}[T] \to \mathbb{C}[T]$ by*

$$\rho(e^{Tu}) = \exp\left(\sum_{n=2}^{\infty} \frac{(-1)^n}{n} \zeta(n) u^n \right) e^{Tu}, \qquad |u| < 1.$$

Then for any index set $(\mathbf{s}|\mathbf{i})$ one has

$$Z^ш_{(\mathbf{s}|\mathbf{i})}(T) = \rho(Z^*_{(\mathbf{s}|\mathbf{i})}(T)). \tag{10}$$

Definition 2.10. Let w be a positive integer such that $w \geq 2$. Let $(\mathbf{s}|\mathbf{i})$ be any index set with the weight of $\mathbf{s}$ equal to w. Then every weight w MPV relation produced by (10) is called a *regularized double shuffle* relation (RDS) of weight w. This is obtained by formally setting $T = 0$ in (10).

Theorem 2.9 is a generalization of [24, Thm. 1] to the higher level MPV cases. The proof is essentially the same. The above steps can be easily transformed to computer codes which are used in our MAPLE programs. For example, one gets by stuffle product

$$\begin{aligned} TL_N(2|3) =& Z^*_{(1|0)}(T) Z^*_{(2|3)}(T) = Z^*(y_{1,0} * y_{2,3}) \\ =& Z^*_{(1,2|0,3)}(T) + Z^*_{(2,1|3,3)}(T) + Z^*_{(3|3)}(T), \end{aligned}$$

while using shuffle product one has

$$\begin{aligned} TL_N(2|3) =& Z^ш_{(1|0)}(T) Z^ш_{(2|3)}(T) = Z^ш(y_{1,0} ш y_{2,3}) = Z^ш(b_0 ш a b_3) \\ =& Z^ш_{(1,2|0,3)}(T) + Z^ш_{(2,1|0,3)}(T) + Z^ш_{(2,1|3,0)}(T). \end{aligned}$$

Hence one discovers the following RDS by comparing the above two expressions using Thm. 2.9:

$$L_N(2,1|3,0) + L_N(3|3) = L_N(2,1|3,N-3) + L_N(2,1|0,3).$$

3 Weight one relations

When $N \geq 4$ there exist linear relations among MPVs of weight one by a theorem of Bass [1]. These relations are important because by multiplying any MPV of weight $w-1$ by such a relation one can get a relation between MPVs of weight w which is called a *weight one relation.* This is one of the key ideas in finding the formula in [17, 5.25] concerning $d(w,N)$.
Clearly, there are $N-1$ MPVs of weight 1 and level N:

$$L_N(1|j) = -\log(1-\mu^j), \qquad 0<j<N,$$

where $\mu = \mu_N = \exp(2\pi\sqrt{-1}/N)$ as before. Here one can take $\mathbb{C} - (-\infty, 0]$ as the principle branch of the logarithm. Further, it follows from the motivic theory of classical polylogs developed by Beilinson and Deligne in [2] and the Borel's theorem (see [20, Thm. 2.1]) that the $\mathbb{Q}$-dimension of $\mathcal{MPV}(1,N)$ is

$$d(1,N) = \dim K_1(\mathbb{Z}[\mu_N][1/N]) \otimes \mathbb{Q} + 1 = \varphi(N)/2 + \nu(N),$$

where φ is the Euler's totient function and $\nu(N)$ is the number of distinct prime factors of N. Hence there are many linear relations among $L_N(1|j)$. For instance, if $j < N/2$ then one has the symmetric relation

$$-\log(1-\mu^j) = -\log(1-\mu^{N-j}) - \log(-\mu^j) = -\log(1-\mu^{N-j}) + \frac{N-2j}{N}\pi\sqrt{-1}.$$

Thus for all $1 < j < N/2$

$$(N-2)(L_N(1|j) - L_N(1|N-j)) = (N-2j)(L_N(1|1) - L_N(1|N-1)). \quad (11)$$

Further, from [1, (B)] for any divisor d of N and $1 \leq a < N/d$ one has the distribution relation

$$\sum_{0\leq j<d} L_N(1|a+jN/d) = L_N(1|ad). \quad (12)$$

It follows from the main result of Bass [1] (corrected by Ennola [18]) that all the linear relations between $L_N(1|j)$ are consequences of (11) and (12). Hence the weight one relations have the following forms in words: for all $w \in \mathfrak{A}^0$

$$\begin{cases} (N-2)Z(y_{1,j} * w - y_{1,-j} * w) = (N-2j)Z(y_{1,1} * w - y_{1,-1} * w), \\ \displaystyle\sum_{0\leq j<d} Z(y_{1,a+jN/d} * w) = Z(y_{1,ad} * w). \end{cases} \quad (13)$$

4 Regularized distribution relations

It is well-known that multiple polylogs satisfy the following distribution formula (cf. [26, Prop. 2.25]):

$$Li_{s_1,\dots,s_n}(x_1,\dots,x_n) = d^{s_1+\dots+s_n-n} \sum_{y_j^d = x_j, 1\leq j\leq n} Li_{s_1,\dots,s_n}(y_1,\dots,y_n), \quad (14)$$

for all positive integer d. When $s_1 = 1$ one has to exclude the divergent case $x_1 = 1$. We call these *finite distribution relations* (FDT). Racinet further considers the regularized version of these relations, which we now recall briefly. Fix an embedding $\boldsymbol{\mu}_N \hookrightarrow \mathbb{C}$ and denote by Γ its image. Define two sets of words

$$\mathbf{X} := \mathbf{X}_\Gamma = \{x_\sigma : \sigma \in \Gamma \cup \{0\}\}, \quad \text{and} \quad \mathbf{Y} := \mathbf{Y}_\Gamma = \{x_0^{n-1} x_\sigma : n \in \mathbb{N}, \sigma \in \Gamma\}.$$

Then one may consider the coproduct Δ of $\mathbb{Q}\langle\mathbf{X}\rangle$ defined by $\Delta x_\sigma = 1 \otimes x_\sigma + x_\sigma \otimes 1$ for all $\sigma \in \Gamma \cup \{0\}$. For every path $\gamma \in \mathbb{P}^1(\mathbb{C}) - (\{0,\infty\} \cup \Gamma)$ Racinet defines the group-like element $\mathcal{I}_\gamma \in \mathbb{C}\langle\langle\mathbf{X}\rangle\rangle$ by

$$\mathcal{I}_\gamma := \sum_{p\in\mathbb{N},\sigma_1,\dots,\sigma_p\in\Gamma\cup\{0\}} \mathcal{I}_\gamma(\sigma_1,\dots,\sigma_p) x_{\sigma_1}\cdots x_{\sigma_p},$$

where $\mathcal{I}_\gamma(\sigma_1,\dots,\sigma_p)$ is the iterated integral $\int_\gamma \omega(\sigma_1)\cdots\omega(\sigma_p)$ with

$$\omega(\sigma)(t) = \begin{cases} \sigma\, dt/(1-\sigma t), & \text{if } \sigma \neq 0; \\ dt/t, & \text{if } \sigma = 0. \end{cases}$$

(One has to correct the obvious typo in the displayed formula just before Prop. 2.8 in [26] by changing a_j to α_j.) This I_γ is essentially the same element denoted by dch in [17]. Note that $\mathbb{Q}\langle\mathbf{Y}\rangle$ is the sub-algebra of $\mathbb{Q}\langle\mathbf{X}\rangle$ generated by words not ending with x_0. Let $\pi_\mathbf{Y} : \mathbb{Q}\langle\mathbf{X}\rangle \to \mathbb{Q}\langle\mathbf{Y}\rangle$ be the projection. As x_0 is a primitive element one quickly deduces that $(\mathbb{Q}\langle\mathbf{Y}\rangle, \Delta)$ has a graded co-algebra structure.

Let $\mathbb{Q}\langle\mathbf{X}\rangle_{\mathsf{cv}}$ be the sub-algebra of $\mathbb{Q}\langle\mathbf{X}\rangle$ not beginning with x_1 and not ending with x_0. Let $\pi_{\mathsf{cv}} : \mathbb{Q}\langle\mathbf{X}\rangle \to \mathbb{Q}\langle\mathbf{X}\rangle_{\mathsf{cv}}$ be the projection. Passing to the limit one gets:

Proposition 4.1. ([26, Prop.2.11]) *The series $\mathcal{I}_{\mathsf{cv}} := \lim_{a\to 0^+, b\to 1^-} \pi_{\mathsf{cv}}(\mathcal{I}_{[a,b]})$ is group-like in $(\mathbb{C}\langle\langle\mathbf{X}\rangle\rangle_{\mathsf{cv}}, \Delta)$.*

Remark 4.2. The algebras $\mathfrak{A}$, $\mathfrak{A}^0$ and $\mathfrak{A}^1$ in §2 are essentially equal to $\mathbb{Q}\langle\mathbf{X}\rangle$, $\mathbb{Q}\langle\mathbf{X}\rangle_{\mathsf{cv}}$ and $\mathbb{Q}\langle\mathbf{Y}\rangle$, respectively, after setting $a = x_0$ and $b_j = x_{\mu^j}$.

Let $\mathcal{I}$ be the unique group-like element in $(\mathbb{C}\langle\langle\mathbf{X}\rangle\rangle, \Delta)$ whose coefficients of x_0 and x_1 are 0 such that $\pi_{\mathsf{cv}}(\mathcal{I}) = \mathcal{I}_{\mathsf{cv}}$. In order to do the numerical computation one needs to determine explicitly the coefficients for $\mathcal{I}$. Put

$$\mathcal{I} = \sum_{p\in\mathbb{N},,\sigma_1,\dots,\sigma_p\in\Gamma\cup\{0\}} C(\sigma_1,\dots,\sigma_p) x_{\sigma_1}\cdots x_{\sigma_p}. \tag{15}$$

Proposition 4.3. *Let p, m and n be three non-negative integers. If $p > 0$ then* *we assume* $\sigma_1 \neq 1$ *and* $\sigma_p \neq 0$. *Set* $(\sigma_1, \dots, \sigma_p, \{0\}^n) = (\sigma_1, \dots, \sigma_q)$. *Then*

$$C(\{1\}^m, \sigma_1, \dots, \sigma_p, \{0\}^n)$$
$$= \begin{cases} 0, & \text{if } mn = p = 0; \\ Z\big(\pi_{\mathsf{cv}}(x_{\sigma_1} \cdots x_{\sigma_p})\big), & \text{if } m = n = 0; \\ -\dfrac{1}{m} \displaystyle\sum_{i=1}^{q} C(\{1\}^{m-1}, \sigma_1, \dots, \sigma_i, 1, \sigma_{i+1}, \dots, \sigma_q), & \text{if } m > 0; \\ -\dfrac{1}{n} \displaystyle\sum_{i=1}^{p} C(\sigma_1, \dots, \sigma_{i-1}, 0, \sigma_i, \dots, \sigma_p, \{0\}^{n-1}), & \text{if } m = 0, n > 0. \end{cases} \tag{16}$$

Here Z *is defined by* (5) *after using the identification given by Remark* 4.2.

Remark 4.4. This proposition provides the recursive relations one may use to compute all the coefficients of $\mathcal{I}$.

Proof. Since $\mathcal{I}$ is group-like one has

$$\Delta \mathcal{I} = \mathcal{I} \otimes \mathcal{I}. \tag{17}$$

The first case follows from this immediately since $C(0) = C(1) = 0$. The second case is essentially the definition (5) of Z. If $m > 0$ then one can compare the coefficient of $x_1 \otimes x_1^{m-1} x_{\sigma_1} \cdots x_{\sigma_q}$ of the two sides of (17) and find the relation (16). Finally, if $m = 0$ and $n > 0$ then one may similarly consider the coefficient of $x_{\sigma_1} \cdots x_{\sigma_p} x_0^{n-1} \otimes x_0$ in (17). This finishes the proof of the proposition. □

For any divisor d of N let $\Gamma^d = \{\sigma^d : \sigma \in \Gamma\}$, $i_d : \Gamma^d \hookrightarrow \Gamma$ the embedding, and $p^d : \Gamma \twoheadrightarrow \Gamma^d$ the dth power map. They induce two algebra homomorphisms:

$$p^d_* : \mathbb{Q}\langle \mathbf{X}_\Gamma \rangle \longrightarrow \mathbb{Q}\langle \mathbf{X}_{\Gamma^d} \rangle$$
$$x_\sigma \longmapsto \begin{cases} d x_0, & \text{if } \sigma = 0, \\ x_{\sigma^d}, & \text{if } \sigma \in \Gamma, \end{cases}$$

and

$$i^*_d : \mathbb{Q}\langle \mathbf{X}_\Gamma \rangle \longrightarrow \mathbb{Q}\langle \mathbf{X}_{\Gamma^d} \rangle$$
$$x_\sigma \longmapsto \begin{cases} x_0, & \text{if } \sigma = 0, \\ x_\sigma, & \text{if } \sigma \in \Gamma^d, \\ 0, & \text{otherwise.} \end{cases}$$

It is easy to see that both i^*_d and p^d_* are Δ-coalgebra morphisms such that $i^*_d(\mathcal{I})$ and $p^d_*(\mathcal{I})$ have the same image under the map π_{cv}. By the standard Lie-algebra mechanism one has

Proposition 4.5. ([26, Prop.2.26]) *For every divisor d of N*

$$p_*^d(\mathcal{I}) = \exp\left(\sum_{\sigma^d=1,\sigma\neq 1} Li_1(\sigma)x_1\right) i_d^*(\mathcal{I}). \tag{18}$$

Combined with Proposition 4.3 the above result provides the so-called *regularized distribution relations* (RDT) which of course include all the FDT of MPVs given by (14).
However, sometimes FDT are not independent of the other relations. In the next theorem one sees that when the weight $w = 2$ and level N is a prime, all the distribution relations in (14), where $x_j = 1$ for all j, are consequences of RDS of MPVs of level N.

Theorem 4.6. *For any prime p write $L(i,j) = L_p(1,1|i,j)$ and $D(i) = L_p(2|i)$. Define for $1 \le i,j < p$:*

$$\mathrm{FDT} := -D(0) + p\sum_{j=0}^{p-1} D(j), \qquad \mathrm{RDS}(i) := D(i) + L(i,0) - L(i,-i),$$
$$\mathrm{FDS}(i,j) := D(i+j) + L(i,j) + L(j,i) - L(i,j-i) - L(j,i-j).$$

Then one has

$$\mathrm{FDT} = \sum_{1\le i<p} \mathrm{FDS}(i,i) + 2\sum_{1\le j<i<p} \mathrm{FDS}(i,j) + 2\sum_{i=1}^{p-1} \mathrm{RDS}(i). \tag{19}$$

Proof. When $p = 2$ the second term on the right hand side of (19) is vacuous. Then it is easy to see that both sides of (19) are equal to $D(0) + 2D(1)$.
We now assume $p \ge 3$. Changing the order of summation yields that

$$\begin{aligned}
&2\sum_{1\le j<i<p} D(i+j) = \sum_{i=2}^{p-1}\sum_{j=1}^{i-1} D(i+j) + \sum_{j=1}^{p-2}\sum_{i=j+1}^{p-1} D(i+j)\\
=&\sum_{i=2}^{p-2}\sum_{i\neq j=1}^{p-1} D(i+j) + \sum_{j=1}^{p-2} D(j-1) + \sum_{i=2}^{p-1} D(i+1)\\
=&(p-3)\sum_{j=0}^{p-1} D(j) - \sum_{i=2}^{p-2} D(i) - \sum_{i=1}^{p-1} D(2i) + \sum_{j=1}^{p-2} D(j) + \sum_{j=2}^{p-1} D(j) + 2D(0)\\
=&(p-1)D(0) + (p-3)\sum_{j=1}^{p-1} D(j)
\end{aligned}$$

since $\sum_{j=0}^{p-1} D(i+j) = \sum_{j=0}^{p-1} D(j)$ for all i and $\sum_{i=1}^{p-1} D(2i) = \sum_{i=1}^{p-1} D(i)$. This implies that the dilogarithms on the right hand side of (19) exactly add up to

FDT. Thus one only needs to show that all the double logarithms on the right hand side of (19) cancel out.

First observe that $L(i,0)$ in FDS(i,i) and RDS(i) cancel out each other. Now let us consider the lattice points (i,j) of $\mathbb{Z}^2$ corresponding to $L(i,j)$. The points (i,j) corresponding to $L(i,j)$ with positive signs fill in exactly the area inside the square $[1,p-1]\times[1,p-1]$ (including boundary): $L(i,i)$ in FDS(i,i) provides the diagonal $y=x$, $\sum_{1\le j<i<p} L(i,j)$ (resp. $\sum_{1\le j<i<p} L(j,i)$) form the lower right (resp. upper left) triangular region.

For the negative terms of the double logs, $L(i,-i)$ in RDS(i) provides the diagonal $x+y=p$, $\sum_{1\le j<i<p} L(i,j-i)=\sum_{i=2}^{p-1}\sum_{j=p+1-i}^{p-1} L(i,j)$ form the upper right triangular region. Similarly, by changing the order of summation $\sum_{1\le j<i<p} L(j,i-j)=\sum_{i=1}^{p-2}\sum_{j=i+1}^{p-1} L(i,j-i)=\sum_{i=1}^{p-2}\sum_{j=1}^{p-1-i} L(i,j)$ fills the lower left region. □

To conclude this section we remark that numerical evidence up to level $N=169$ supports the following

Conjecture 4.7. *In weight two, all RDT are consequences of the weight one relations, RDS and depth two FDT.*

5 Lifted relations from lower weights

Note that when $N=3$ there are no weight one relations nor (regularized) distribution relations. When we deal with MZVs (resp. alternating Euler sums) we expect that all the linear relations come from RDS (resp. RDS and RDT). Since there is no weight one relation when level $N\le 3$ it is natural to ask if RDS and RDT are enough when $N=3$. Surprisingly, the answer is no.

The first counterexample is in weight four, i.e., $(w,N)=(4,3)$. Easy computation shows that there are 144 MPVs in this case among which there are 239 nontrivial RDS of weight four which include 191 FDS of weight four (see (9) and (10)). Furthermore, it is easy to verify that all the seven RDT (including four FDT) can be derived from RDS. Using these relations we get 127 independent linear relations among the 144 MPVs. But we have $d(4,3)\le 16$ by [17, 5.25], so there must be at least one more linearly independent relation. Where else can we find it? The answer is the so-called *lifted relations.*.

We know that a product of two weight two MPVs is of weight four. So on each of the five RDS (including two FDS) of weight two in $\mathcal{MPV}(2,3)$ we can multiply any one of the nine MPVs of $(w,N)=(2,3)$ to get a relation in $\mathcal{MPV}(4,3)$. For instance, we have a FDS

$$Z(y_{1,1}*y_{1,1}-y_{1,1}ш y_{1,1})=L_3(2|2)+2L_3(1,1|1,1)-L_3(1,1|1,0)=0.$$

Multiplying by $L_3(1,1|1,1)=Z(y_{1,1}y_{1,2})$ we obtain a new relation which is linearly independent from RDS of weight four in $\mathcal{MPV}(4,3)$:

$$\begin{aligned}
&Z\big(y_{1,1}y_{1,2}ш(y_{2,0}+2y_{1,1}y_{1,2}-2y_{1,1}y_{1,0})\big)\\
=&L_3(1,1,2|1,1,0)+2L_3(1,2,1|1,1,0)+2L_3(2,1,1|1,1,0)\\
+&L_3(2,1,1|2,2,1)+4L_3(\{1\}^4|1,1,2,1)+8L_3(\{1\}^4|1,0,1,0)\\
-&6L_3(\{1\}^4|1,0,0,1)-4L_3(\{1\}^4|1,0,1,2)-2L_3(\{1\}^4|1,1,2,0)=0.
\end{aligned}$$

Such relations coming from the lower weights are called *lifted relations.* In this way, when $(w,N)=(4,3)$ we can produce 45 lifted RDS relations from weight two, 58 from weight three. We may also lift RDT and obtain nine and six relations from weight two and three, respectively. However, all the lifted relations together only produce one new linearly independent relation, as expected. Hence we find totally 128 linearly independent relations among the 144 MPVs with $(w,N)=(4,3)$. This implies that $d(4,3)\le 16$ which is the same bound obtained by [17, 5.25] and is proved to be exact under a variant of Grothendieck's period conjecture by Deligne [16].
For levels $N\ge 4$ one may lift not only RDS and RDT but also the weight one relations. But by a moment reflection one sees that the lifted weight one relations are still weight one relations by themselves so one doesn't really need to consider them after all.

Definition 5.1. We call a $\mathbb{Q}$-linear relation among MPVs *standard* if it can be produced by some $\mathbb{Q}$-linear combinations of the following four families of relations: regularized double shuffle relations, regularized distribution relations, weight one relations, and lifted relations from the above. Otherwise, it is called a *non-standard* relation.

In general, there are no inclusion relations among the four families of the standard relations.
Computation in small weight cases supports the following

Conjecture 5.2. *Suppose $N=3$ or 4. Every MPV of level N is a linear combination of MPVs of the form $L(\{1\}^w|t_1,\dots,t_w)$ with $t_j\in\{1,2\}$. Consequently, the $\mathbb{Q}$-dimension of the MPVs of weight w and level N is given by $d(w,N)=2^w$ for all $w\ge 1$.*

Remark 5.3. The data in Table 2 in §7 shows that one cannot produce enough relations by using only the standard relations when $(w,N)=(3,4)$. In fact, even though one has $d(3,4)\le 8$ and $d(4,4)\le 16$ by [17, 5.25], one can only show that $d(3,4)\le 9$ and $d(4,4)\le 21$ by using only the standard relations. However, thanks to the octahedral symmetry of $\mathbb{P}^1-(\{0,\infty\}\cup\boldsymbol{\mu}_4)$ one can find (presumably all) the non-standard relations in these two cases (see Thm. 9.1).
Remark 5.4. Let $N=2,3,4$ or 8. Assuming a variant of Grothendieck's period conjecture, Deligne [16] constructed explicitly a set of basis for $\mathcal{MPV}(w,N)$. His results would also imply that $d(w,2)$ is given by the Fibonacci numbers, $d(w,3)=d(w,4)=2^w$, and $d(w,8)=3^w$ under Grothendieck's period conjecture.

6 Some conjectures of FDS and RDS

Fix a level N. Let R be a commutative $\mathbb{Q}$-algebra with 1 and a homomorphism $Z_R : \mathfrak{A}^0 \longrightarrow R$ such that the *finite double shuffle* (FDS) property holds:

$$Z_R(\omega_1 ш \omega_2) = Z_R(\omega_1 * \omega_2) = Z_R(\omega_1)Z_R(\omega_2).$$

We then extend Z_R to $Z_R^{ш}$ and Z_R^* as before. Define an R-module automorphism ρ_R of $R[T]$ by

$$\rho_R(e^{Tu}) = A_R(u)e^{Tu}$$

where

$$A_R(u) = \exp\left(\sum_{n=2}^{\infty} \frac{(-1)^n}{n} Z_R(a^{n-1}b_0)u^n\right) \in R[\![u]\!].$$

If a map $Z_R : \mathfrak{A}^0 \longrightarrow R$ satisfies the FDS and $(Z_R^{ш} - \rho_R \circ Z_R^*)(\omega) = 0$ for all $\omega \in \mathfrak{A}^1$ then we say that Z_R has the *regularized double shuffle* (RDS) property. Let R_{RDS} be the universal algebra (together with a map $Z_{RDS} : \mathfrak{A}^0 \longrightarrow R_{RDS}$) such that for every $\mathbb{Q}$-algebra R and a map $Z_R : \mathfrak{A}^0 \longrightarrow R$ satisfying RDS there always exists a map φ_R to make the following diagram commutative:

$$\begin{array}{ccc} \mathfrak{A}^0 & \xrightarrow{Z_{RDS}} & R_{RDS} \\ & \searrow^{Z_R} & \downarrow \varphi_R \\ & & R \end{array}$$

When $N = 2$ computation by Blümlein, Broadhurst and Vermaseren [5] shows that the finite distribution relations and the regularized distribution relations (18) contribute non-trivially when the weight $w = 8$ and $w = 11$, respectively. When $N = 3$ computation shows that the lifted relations contribute non-trivially when the weight $w = 4$ (see §5) and $w = 5$: we can only get $d(5,3) \le 33$ instead of the conjecturally correct dimension 32 without using the lifted relations. Note that in this case there are 612 FDS of weight five, 191 RDS of weight five, 8 FDT and 7 RDT.

One may use the fact that Z_R is an algebra homomorphism to produce *lifted finite double shuffle* and *lifted regularized double shuffle* relations as follows: for all $\omega_1 \in \mathfrak{A}^1$, $\omega_0, \omega_0', \omega_0'' \in \mathfrak{A}^0$ with $\lg(\omega_1) + \lg(\omega_0) = \lg(\omega_0) + \lg(\omega_0') + \lg(\omega_0'') = w$

$$Z_R^{ш}(\omega_1 ш \omega_0) - \rho_R \circ Z_R^*(\omega_1) Z_R^{ш}(\omega_0) = 0, \quad Z_R\big((\omega_0 * \omega_0') * \omega_0'' - (\omega_0 ш \omega_0') * \omega_0''\big) = 0.$$

In general, one can define the universal objects Z_{SR} and R_{SR} corresponding to the standard relations similar to Z_{RDS} and R_{RDS} such that for every $\mathbb{Q}$-algebra R and a map $Z_R : \mathfrak{A}^0 \longrightarrow R$ satisfying the standard relations there always exists a map φ_R to make the following diagram commutative:

$$\begin{array}{ccc} \mathfrak{A}^0 & \xrightarrow{Z_{SR}} & R_{SR} \\ & \searrow^{Z_R} & \downarrow \varphi_R \\ & & R \end{array} \qquad (20)$$

Recall that one has the evaluation map $Z : \mathfrak{A}^0 \longrightarrow \mathbb{C}$ by Prop. 2.8 which extends (5).

Conjecture 6.1. *Let* $(R, Z_R) = (\mathbb{R}, Z)$ *if* $N = 1$, *and* $(R, Z_R) = (\mathbb{C}, Z)$ *if* $N = 2, 3$ *or* $N = p^n$ *with prime* $p \geq 5$. *If* $N = 1$ *(resp.* $N = 2$*) then the map* $\varphi_{\mathbb{R}}$ *is injective, namely, the algebra of MPVs of level one or two is isomorphic to* R_{RDS} *(resp.* R_{SR}*). If* $N = 3$ *or* $N = p^n$ $(p \geq 5)$ *then the map* $\varphi_{\mathbb{C}}$ *is injective so the algebra of MPVs of level* N *is isomorphic to* R_{SR}.

The above conjecture generalizes [24, Conjecture 1]. It means that all the linear relations among MPVs can be produced by RDS when $N = 1$ or 2, and by the standard ones when $N = 3$ or p^n with prime $p \geq 5$. When $N = p \geq 5$, p a prime, this is proved in Thm. 8.6 under the assumption of a variant of Grothendieck's period conjecture.

Computation in many cases such as those listed in Remark 8.2 and Conjecture 8.5 show that MPVs must satisfy some other relations apart from the standard ones when N has at least two distinct prime factors, so a naive generalization of Conjecture 6.1 to all levels does not exist at present. However, when $N = 4$ one can show that octahedral symmetry of $\mathbb{P}^1 - (\{0, \infty\} \cup \boldsymbol{\mu}_4)$ provide all the non-standard relations under the standard assumption (see Thm. 9.1). But since we only have numerical evidence in weight three and weight four it may be a little premature to form a conjecture for level four.

7 The structure of MPVs and some examples

In this section we concentrate on RDS between MPVs of small weights. Most of the computations in this section are carried out by MAPLE. We have checked the consistency of these relations with many known ones and verified our results numerically using GiNac [27] and EZ-face [9].

By considering all the admissible words we see easily that the number of distinct MPVs of weight $w \geq 2$ and level N is $N^2(N+1)^{w-2}$ and there are at most $N(N+1)^{w-2}$ RDS (but not FDS). If $w \geq 4$ then the number of FDS is given by

$$(N-1)N^2(N+1)^{w-3} + \Big(\Big[\frac{w}{2}\Big] - 1\Big) N^4 (N+1)^{w-4} = \Big(N^2\Big[\frac{w}{2}\Big] - 1\Big) N^2 (N+1)^{w-4}.$$

If $w = 2$ (resp. $w = 3$) then the number of FDS is $(N-1)^2$ (resp. $N^2(N-1)$). Therefore, it is not hard to see that the number of standard relations grow polynomially with the level N but exponentially with the weight w.

7.1 Weight one

From §3 we know that all relations in weight one follow from (11) and (12), and no RDS exists. The relations in weight one are crucial for higher level cases because they provide the weight one relations considered in §3. Moreover, easy computation by (11) and (12) shows that there is a hidden integral structure, namely, in each level there exists a $\mathbb{Q}$-basis consisting of MPVs such that every other MPV is a $\mathbb{Z}$-linear combination of the basis elements. This fact is proved by Conrad [13, Theorem 4.6]. Similar results should hold for higher weight cases and we hope to return to this in a future publication [14].

7.2 Weight two

There are N^2 MPVs of weight two and level N:

$$L_N(1,1|i,j), \quad L_N(2|j), \qquad 1 \le i \le N-1, 0 \le j \le N-1.$$

For $1 \le i,j < N$ the FDS $Z^*(y_{1,i} * y_{1,j}) = Z^{\text{III}}(y_{1,i} ш y_{1,j})$ yields

$$L_N(2|i+j) + L_N(1,1|i,j) + L_N(1,1|j,i) = L_N(1,1|i,j-i) + L_N(1,1|j,i-j). \tag{21}$$

Now from RDS $\rho(Z^*(y_{1,0} * y_{1,i})) = Z^{\text{III}}(y_{1,0} ш y_{1,i})$ we get for $1 \le i < N$

$$L_N(1,1|i,0) + L_N(2|i) = L_N(1,1|i,-i). \tag{22}$$

The FDT in (14) yields: for every divisor d of N, and $1 \le a,b < d' := N/d$

$$L_N(2|ad) = d \sum_{j=0}^{d-1} L_N(2|a+jd'), \tag{23}$$

$$L_N(1,1|ad,bd) = \sum_{j,k=0}^{d-1} L_N(1,1|a+jd',b+kd'). \tag{24}$$

To derive the RDT we can compare the coefficients of $x_1 x_{\mu^{ad}}$ in (18) and use Prop. 4.3 to get: for every divisor d of N, and $1 \le a < d'$

$$L_N(1|ad) \sum_{j=1}^{d-1} L_N(1|jd') = \sum_{j=1}^{d-1} \sum_{k=0}^{d-1} L_N(1,1|jd',a+kd') - \sum_{k=0}^{d-1} L_N(1,1|a+kd',-a-kd') - L_N(1,1|ad,-ad). \tag{25}$$

By definition, the weight one relations are obtained from (11) and (12). For example, if $N = p$ is a prime then (12) is trivial and (11) is equivalent to the following: for all $1 \le j < h$ ($h := (p-1)/2$)

$$L_N(1|j) - L_N(1|-j) = (p-2j)(L_N(1|h) - L_N(1|h+1)). \tag{26}$$

Thus multiplying by $L_N(1|i)$ ($1 \le i < p$) and applying the shuffle relation $L_N(1|a)L_N(1|b) = L_N(1^2|a,b-a) + L_N(1^2|b,a-b)$ (here we put $L_N(1^2|-) = L_N(1,1|-)$ to save space) we get:

$$L_N(1^2|i,j-i) + L_N(1^2|j,i-j) - L_N(1^2|i,-j-i) - L_N(1^2|-j,i+j) = (p-2j)\big(L_N(1^2|i,h-i) + L_N(1^2|h,i-h) - L_N(1^2|i,-i-h) - L_N(1^2|-h,i+h)\big). \tag{27}$$

Computation shows that the following conjecture should hold.

Conjecture 7.1. *The RDT* (25) *follows from the combination of the following relations: the weight one relations, the RDS* (21) *and* (22)*, and the FDT* (23) *and* (24).

7.3 Weight three

Apparently there are $N^2(N+1)$ MPVs of weight three and level N: for each choice (i,j,k) with $1 \le i \le N-1, 0 \le j,k \le N-1$ we have four MPVs of level N:

$$L_N(1^3|i,j,k) := L_N(1,1,1|i,j,k), \quad L_N(1,2|i,j), \quad L_N(2,1|j,k), \quad L_N(3|k).$$

For $1 \le i,j,k < N$ the FDS $Z^*\big(y_{1,i} * (y_{1,j}y_{1,k})\big) = Z^{\text{Ш}}\big(y_{1,i}\text{ш}(y_{1,j}y_{1,k})\big)$ yields

$$\begin{aligned} L_N(1^3|i,j-i,k) + L_N(1^3|j,i-j,k+j-i) + L_N(1^3|j,k,i-k-j) \\ = L_N(2,1|i+j,k) + L_N(1,2|j,i+k) \\ + L_N(1^3|i,j,k) + L_N(1^3|j,i,k) + L_N(1^3|j,k,i). \end{aligned} \tag{28}$$

For $1 \le i,j < N$ the FDS $Z^*(y_{1,i} * y_{2,j}) = Z^{\text{Ш}}(y_{1,i}\text{ш}y_{2,j})$ yields

$$\begin{aligned} L_N(3|i+j) + L_N(1,2|i,j) + L_N(2,1|j,i) \\ = L_N(1,2|i,j-i) + L_N(2,1|i,j-i) + L_N(2,1|j,i-j). \end{aligned} \tag{29}$$

Moreover, there are three ways to produce RDS. Since $\rho(T) = T$ the first family of RDS come from $Z^*\big(y_{1,0} * (y_{1,i}y_{1,i+j})\big) = Z^{\text{Ш}}\big(y_{1,0}\text{ш}(y_{1,i}y_{1,i+j})\big)$ for $1 \le i \le N-1, 0 \le j \le N-1$:

$$\begin{aligned} y_{1,0} * (y_{1,i}y_{1,i+j}) &= y_{1,0}y_{1,i}y_{1,i+j} + y_{1,i}\tau_i(y_{1,0} * y_{1,j}) + y_{2,i}y_{1,i+j} \\ =& y_{1,0}y_{1,i}y_{1,i+j} + y_{1,i}y_{1,i}y_{1,i+j} + y_{1,i}y_{1,i+j}y_{1,i+j} + y_{1,i}y_{2,i+j} + y_{2,i}y_{1,i+j} \end{aligned}$$

On the other hand,

$$y_{1,0}\text{ш}y_{1,i}y_{1,i+j} = y_{1,0}y_{1,i}y_{1,i+j} + y_{1,i}y_{1,0}y_{1,i+j} + y_{1,i}y_{1,i+j}y_{1,0}.$$

Hence

$$\begin{aligned} L_N(1^3|i,0,j) + L_N(1^3|i,j,0) + L_N(1,2|i,j) + L_N(2,1|i,j) \\ = L_N(1^3|i,-i,i+j) + L_N(1^3|i,j,-i-j). \end{aligned} \tag{30}$$

The second family of RDS follow from $\rho(Z^*(y_{1,0} * y_{2,i})) = Z^{\text{Ш}}(y_{1,0}\text{ш}y_{2,i})$:

$$y_{1,0}y_{2,i} + y_{2,i}y_{1,i} + y_{3,i} = y_{1,0}y_{2,i} + y_{2,0}y_{1,i} + y_{2,i}y_{1,0}$$

which implies that

$$L_N(2,1,i,0)+L_N(3,i)=L_N(2,1,i,-i)+L_N(2,1,0,i). \tag{31}$$

Now we consider the last family of RDS. By the definition of stuffle product:

$$\begin{aligned} y_{1,0}*y_{1,0}*y_{1,i} =&(2y_{1,0}^2+y_{2,0})*y_{1,i}\\ =&2y_{1,0}(y_{1,0}*y_{1,i})+2y_{1,i}^3+2y_{2,i}y_{1,i}+y_{2,0}*y_{1,i}\\ =&2y_{1,0}^2y_{1,i}+2y_{1,0}y_{1,i}^2+2y_{1,0}y_{2,i}+2y_{1,i}^3+2y_{2,i}y_{1,i}+y_{2,0}*y_{1,i}. \end{aligned}$$

Applying $\rho\circ Z^*$ and noticing that $Z^{ш}_{(2|0)}(T)=\zeta(2)$ we get

$$\begin{aligned} (T^2+\zeta(2))Z^{ш}_{(1|i)}(T)=&2Z^{ш}_{(1^3|0,0,i)}(T)+2Z^{ш}_{(1^3|0,i,i)}(T)+2Z^{ш}_{(1,2|0,i)}(T)\\ &+2Z^{ш}_{(1^3|i,i,i)}(T)+2Z^{ш}_{(2,1|i,i)}(T)+Z^{ш}_{(2|0)}(T)Z^{ш}_{(1|i)}(T). \end{aligned} \tag{32}$$

On the other hand by the definition of shuffle product

$$y_{1,0}ш y_{1,0}ш y_{1,i}=2y_{1,0}^2ш y_{1,i}=2y_{1,0}^2y_{1,i}+2y_{1,0}y_{1,i}y_{1,0}+2y_{1,i}y_{1,0}^2$$

Applying $Z^{ш}$ we get

$$T^2Z^{ш}_{(1|i)}(T)=2Z^{ш}_{(1^3|0,0,i)}(T)+2Z^{ш}_{(1^3|0,i,0)}(T)+2Z^{ш}_{(1^3|i,0,0)}(T). \tag{33}$$

We further have

$$\begin{aligned} &Z^{ш}(y_{1,0}y_{1,i}^2+y_{1,0}y_{2,i}-y_{1,0}y_{1,i}y_{1,0})\\ =&Z^{ш}(1^3|0,i,i)(T)+Z^{ш}_{(1,2|0,i)}(T)-Z^{ш}_{(1^3|0,i,0)}(T)\\ =&2Z^{ш}_{(1^3|i,0,0)}(T)-Z^{ш}_{(2,1|i,0)}(T)-Z^{ш}_{(2,1|0,i)}(T)-Z^{ш}_{(1^3|i,0,i)}(T)-Z^{ш}_{(1^3|i,i,0)}(T) \end{aligned}$$

where we have used the facts that

$$\begin{aligned} Z^{ш}_{(1,2|0,i)}(T)=&TZ^{ш}_{(2|i)}(T)-Z^{ш}_{(2,1|i,0)}(T)-Z^{ш}_{(2,1|0,i)}(T)\\ Z^{ш}_{(1^3|0,i,i)}(T)=&TZ^{ш}_{(1,1|i,i)}(T)-Z^{ш}_{(1^3|i,0,i)}(T)-Z^{ш}_{(1^3|i,i,0)}(T)\\ Z^{ш}_{(1^3|0,i,0)}(T)=&TZ^{ш}_{(1,1|i,0)}-2Z^{ш}_{(1^3|i,0,0)}(T)\\ Z^{ш}_{(1,1|i,0)}(T)=&Z^{ш}_{(2|i)}(T)+Z^{ш}_{(1,1|i,i)}(T). \end{aligned}$$

Hence for $1\le i<N$ we have by subtracting (33) from (32)

$$\begin{aligned} L_N(1^3|i,0,0)+L_N(2,1|i,0)+L_N(1^3|i,-i,0)=&\\ L_N(2,1|i,-i)+L_N(2,1|0,i)+L_N(1^3|i,-i,i)&+L_N(1^3|i,0,-i). \end{aligned} \tag{34}$$

Setting $j=0$ in (30) and subtracting from (34) we get

$$L_N(1^3|i,-i,0)=L_N(2,1|i,-i)+L_N(2,1|0,i)+L_N(1^3|i,0,0)+L_N(1,2|i,0). \tag{35}$$

7.4 Upper bound of $d(w,N)$ by Deligne and Goncharov

By using the theory of motivic fundamental groups of $\mathbb{P}^1 - (\{0,\infty\} \cup \boldsymbol{\mu}_N)$ Deligne and Goncharov [17, 5.25] show that $d(w,N) \le D(w,N)$ where $D(w,N)$ are defined by the formal power series

$$1 + \sum_{w=1}^{\infty} D(w,N)t^w = \begin{cases} (1-t^2-t^3)^{-1}, & \text{if } N=1; \\ (1-t-t^2)^{-1}, & \text{if } N=2; \\ (1-at+bt^2)^{-1}, & \text{if } N\ge 3, \end{cases} \tag{36}$$

where $a = a(N) := \varphi(N)/2 + \nu(N)$, $b = b(N) := \nu(N) - 1$, φ is the Euler's totient function and $\nu(N)$ is the number of distinct prime factors of N. If $N > 2$ then we have

$$\sum_{w=1}^{\infty} D(w,N)t^w = at + (a^2-b)t^2 + (a^3-2ab)t^3 + (a^4-3a^2b+b^2)t^4 + \cdots$$

In particular, if p is a prime then for any positive integer n

$$D(w,p^n) = a(p^n)^w = \left(\frac{p^{n-1}(p-1)}{2} + 1\right)^w. \tag{37}$$

We will compare the bound obtained by the standard relations to the bound $D(w,N)$ in the next two sections.

8 Computational results in weight two

In this section we combine the analysis in the previous sections and the theory developed by Deligne and Goncharov [17] to present a detailed computation in weight two and level $N \le 169$.
Let $\mathcal{G} := \iota(\mathrm{Lie}\, U_\omega)$ be the motivic fundamental Lie algebra (see [17, (5.12.2)]) associated to the motivic fundamental group of $\mathbb{P}^1 - (\{0,\infty\} \cup \boldsymbol{\mu}_N)$. As pointed out in §6.13 of op. cit. one may safely replace $\mathcal{G}(\boldsymbol{\mu}_N)^{(\ell)}$ by $\mathcal{G}$ throughout [20]. Then it follows from the proof of [17, 5.25] that if conjecture [17, 5.27(c)] is true, which we assume in the following, then

$$d(2,N) = D(2,N) - \dim\ker(\beta_N), \tag{38}$$

where $\beta_N : \bigwedge^2 \mathcal{G}_{-1,-1} \longrightarrow \mathcal{G}_{-2,-2}$ is given by Ihara's bracket $\beta_N(a\wedge b) = \{a,b\}$ defined by (5.13.6) of op. cit. Here $\mathcal{G}_{\bullet,\bullet}$ is the associated graded of the weight and depth gradings of $\mathcal{G}$ (see [20, §2.1]). Let $k(N) := \dim\ker(\beta_N)$. Then

$$\delta_1(N) := \dim \mathcal{G}_{-1,-1} = \begin{cases} 1, & \text{if } N=1 \text{ or } 2; \\ \varphi(N)/2 + \nu(N) - 1, & \text{if } N \ge 3, \end{cases} \tag{39}$$

by [20, Thm. 2.1]. Thus

$$i(N) := \dim \mathrm{Im}(\beta_N) = \delta_1(N)(\delta_1(N)-1)/2 - k(N). \tag{40}$$

N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
δ_1	1	1	1	1	2	2	3	2	3	3	5	3	6	4	5	4
i	0	0	0	0	0	1	1	1	3	3	5	3	8	6	10	6
k	0	0	0	0	1	0	2	0	0	0	5	0	7	0	0	0
δ_2	0	0	1	1	2	2	4	3	6	5	10	5	14	9	14	10
sr	0	0	1	1	2	2	4	4	6	6	10	8	14	12	16	16
D	1	2	4	4	9	8	16	9	16	15	36	15	49	24	35	25
SR	1	2	4	4	8	8	14	10	16	16	31	18	42	27	37	31
d	1	2	4	4	8	8	14	9	16	15	31	15	42	24	35	25

N	17	18	19	20	21	22	23	24	25	26	27	28	29
δ_1	8	4	9	5	7	6	11	5	10	7	9	7	14
i	16	6	21	10	21	15	33	10	40	21	36	21	56
k	12	0	15	0	0	0	22	0	5	0	0	0	35
δ_2	24	9	30	14	27	20	44	14	50	27	45	27	70
sr	24	18	30	24	32	30	44	32	50	42	54	48	70
D	81	24	100	35	63	48	144	35	121	63	100	63	225
SR	69	33	85	45	68	58	122	53	116	78	109	84	190
d	69	24	85	35	63	48	122	35	116	63	100	63	190

N	30	31	32	33	34	35	36	37	38	39	40	41
δ_1	6	15	8	11	9	13	7	18	10	13	9	20
i	15	65	28	55	36	78	21	96	45	78	36	120
k	0	40	0	0	0	0	0	57	0	0	0	70
δ_2	19	80	36	65	44	90	27	114	54	90	44	140
sr	48	80	64	80	72	96	72	114	90	112	96	140
D	47	256	81	143	99	195	63	361	120	195	99	441
SR	76	216	109	158	127	201	108	304	156	217	151	371
d	47	216	81	143	99	195	63	304	120	195	99	371

N	42	43	44	45	46	47	48	49	121	125	169
δ_1	8	21	11	13	12	23	9	21	55	50	78
i	28	133	55	78	66	161	36	175	1155	1200	2288
k	0	77	0	0	0	92	0	35	330	25	715
δ_2	34	154	65	90	77	184	44	196	1210	1250	2366
sr	96	154	120	144	132	184	128	196	1210	1250	2366
D	79	484	143	195	168	576	99	484	3136	2601	6241
SR	141	407	198	249	223	484	183	449	2806	2576	5526
d	79	407	143	195	168	484	99	449	2806	2576	5526

Table 1: Upper bounds of $d(2,N)$ by the standard relations and [17, 5.25].

Since $\dim \mathcal{G}_{-2,-1} = \varphi(N)/2$ if $N > 2$ and 0 otherwise the dimension of the degree two part of $\mathcal{G}$ is

$$\delta_2(N) := \dim \mathcal{G}_{-2,-1} + \dim \mathcal{G}_{-2,-2} = \begin{cases} i(N), & \text{if } N = 1 \text{ or } 2; \\ \varphi(N)/2 + i(N), & \text{if } N \geq 3. \end{cases} \tag{41}$$

Let $sr(N)$ be the upper bound of $\delta_2(N)$ obtained by the standard relations. This can be computed by the method described in [30, §2]. Let $SR(N)$ be the upper bound of $d(2, N)$ similarly obtained by the standard relations. In Table 1 we use MAPLE to provide the following data: $k(N)$, $sr(N)$, and $SR(N)$. Then we can calculate $\delta_1(N)$, $i(N)$ and $\delta_2(N)$ by (39), (40) (41), respectively. From (38) we can check the consistency by verifying

$$sr(N) - \delta_2(N) = SR(N) - d(2, N) = SR(N) - D(2, N) + k(N)$$

which gives the number of linearly independent non-standard relations (assuming the conjecture in [17, 5.27(c)]). In Table 1 we provide some computational data of the above quantities. To save space we write $D = D(2, N)$ and $d = d(2, N)$.

Definition 8.1. We call the level N *standard* if either (i) $N = 1, 2$ or 3, or (ii) N is a prime power p^n ($p \geq 5$). Otherwise N is called *non-standard*.

Remark 8.2. We now make the following comments in the weight two case from Table 1.
(a) When $p \geq 11$ the vector space $\ker \beta_p$ contains a subspace isomorphic to the space of cusp forms of weight two on $X_1(p)$ which has dimension $(p-5)(p-7)/24$ (see [20, Lemma 2.3 & Theorem 7.8]). So it must contain another piece which has dimension $(p-3)/2$ since $\dim(\ker \beta_p) = (p^2 - 1)/24$ by [30, (6)]. One may wonder if this missing piece has any significance in geometry and/or number theory.
(b) If N is a 2-power or a 3-power then $D(2, N)$ should be sharp. See Remark 5.4.
(c) If N has at least two distinct prime factors then $D(2, N)$ seems to be sharp, though we don't have any theory to support it.
(d) Suppose the conjecture in [17, 5.27(c)] is true. Then by [17, 5.27], (b) and (c) is equivalent to saying that the kernel of β_N is trivial if the level N is non-standard. We believe this is also a necessary condition on N for β_N to be trivial.
(e) If the level $N > 3$ is standard then β_N is *unlikely* to be injective. We conjecture that non-standard relation doesn't exist (i.e., $SR(N)$ is sharp), though for prime power levels we only have verified this for the first four prime square levels $N = 5^2, 7^2, 11^2, 13^2$, and the first cubic power level $N = 5^3$.

The equation $\dim \beta_p = (p^2 - 1)/24$ (see [30, (6)]) together with Theorem 8.6 confirms Remark 8.2(e) for prime levels if we assume a variant of Grothendieck's period conjecture [17, 5.27(c)]. The next result partially confirms Remark 8.2(e) in the case when the level is a prime square.

Theorem 8.3. *If $p \geq 5$ is a prime then* $\ker \beta_{p^2} \neq 0$ *and*

$$d(2,p^2) < D(2,p^2) = (p^2-p+2)^2/4.$$

Proof. By the proof of Delign-Goncharov's bound $D(2,p^2)$ in [17, 5.25] we only need to show $\ker \beta_{p^2} \neq 0$. In the following we adopt the same notation as in [17] and [30].

Fix a primitive p^2th root of unity μ. Put $e(a) = e_{\mu^a}$ for all integer a. Define

$$g_{k,j} = e(pk+j) + e(p^2-pk-j) + e(pj) + e(p^2-pj)$$

for $0 \leq k < (p-1)/2$, $1 \leq j \leq p-1$, and for $k=(p-1)/2$, $1 \leq j \leq (p-1)/2$. One only needs to prove the following

Claim. Let $h = (p-3)/2$. Then one has

$$\begin{aligned}
&\sum_{k=0}^{h}\sum_{l=k}^{h}\sum_{j=2}^{p-2}\{g_{k,1},g_{l,j}\} + \sum_{k=0}^{h+1}\sum_{j=2}^{h+1}\{g_{k,1},g_{h+1,j}\}\\
&+\sum_{k=0}^{h}\sum_{l=k+1}^{h}\sum_{j=2}^{p-2}\{g_{k,p-1},g_{l,j}\} + \sum_{k=0}^{h}\sum_{j=2}^{h+1}\{g_{k,p-1},g_{h+1,j}\}\\
&-\sum_{k=0}^{h}\sum_{l=k}^{h}\sum_{j=2}^{p-2}\{g_{k,j},g_{l,p-1}\} - \sum_{k=0}^{h}\sum_{l=k}^{h}\sum_{j=2}^{p-2}\{g_{k,j},g_{l+1,1}\} = 0.
\end{aligned}$$

There are $h(2h+3)^2 = hp^2$ distinct terms on the left, each with coefficient ± 1.

The proof of the claim is straight-forward by a little tedious change of indices and regrouping.

$$-\sum_{k=0}^{h}\sum_{l=k}^{h}\sum_{j=2}^{p-2}\{g_{k,j},g_{l+1,1}\} = \sum_{k=0}^{h}\sum_{l=0}^{k}\sum_{j=2}^{p-2}\{g_{k+1,1},g_{l,j}\} = \sum_{k=1}^{h+1}\sum_{l=0}^{k-1}\sum_{j=2}^{p-2}\{g_{k,1},g_{l,j}\}.$$

Then the expression in the claim becomes

$$\begin{aligned}
&\sum_{k=1}^{h}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,1},g_{l,j}\} + \sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{0,1},g_{l,j}\} + \sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{h+1,1},g_{l,j}\}\\
&+\sum_{k=0}^{h+1}\sum_{j=2}^{h+1}\{g_{k,1},g_{h+1,j}\} + \sum_{k=0}^{h}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,p-1},g_{l,j}\} + \sum_{k=0}^{h}\sum_{j=2}^{h+1}\{g_{k,p-1},g_{h+1,j}\}\\
&=\sum_{k=0}^{h+1}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,1},g_{l,j}\} + \sum_{k=0}^{h+1}\sum_{j=2}^{h+1}\{g_{k,1},g_{h+1,j}\}\\
&+\sum_{k=0}^{h}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,p-1},g_{l,j}\} + \sum_{k=0}^{h}\sum_{j=2}^{h+1}\{g_{k,p-1},g_{h+1,j}\}.
\end{aligned}$$

Let us write $\{a,b\} = \{e(a),e(b)\}$. By definition

$$
\begin{aligned}
&\{g_{k,1}, g_{l,j}\}\\
=&\{pk+1, pl+j\} + \{-pk-1, pl+j\} + \{p, pl+j\} + \{-p, pl+j\}\\
&+\{pk+1, -pl-j\} + \{-pk-1, -pl-j\} + \{p, -pl-j\} + \{-p, -pl-j\}\\
&+\{pk+1, pj\} + \{-pk-1, pj\} + \{p, pj\} + \{-p, pj\}\\
&+\{pk+1, -pj\} + \{-pk-1, -pj\} + \{p, -pj\} + \{-p, -pj\}\\
=&\{pk+1, pl+j\} + \{p(p-k)-1, pl+j\} + \{p, pl+j\} + \{-p, pl+j\}\\
&+\{pk+1, p(p-1-l)+p-j\} + \{p(p-k)-1, p(p-1-l)+p-j\}\\
&\qquad + \{p, p(p-1-l)+p-j\} + \{-p, p(p-1-l)+p-j\}\\
&+\{pk+1, pj\} + \{p(p-k)-1, pj\} + \{p, pj\} + \{-p, pj\}\\
&+\{pk+1, p(p-j)\} + \{p(p-k)-1, p(p-j)\} + \{p, p(p-j)\} + \{-p, p(p-j)\}.
\end{aligned}
$$

Then

$$
\begin{aligned}
&\sum_{k=0}^{h+1}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,1}, g_{l,j}\} = \sum_{k=0}^{h+1}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{pk+1, pl+j\} + \{p(p-k)-1, pl+j\}\\
&+\{pk+1, p(p-1-l)+j\} + \{p(p-k)-1, p(p-1-l)+j\}\\
&+\{p, pl+j\} + \{-p, pl+j\} + \{p, p(p-1-l)+j\} + \{-p, p(p-1-l)+j\}\\
&+2\{pk+1, pj\} + 2\{p(p-k)-1, pj\} + 2\{p, pj\} + 2\{-p, pj\}\\
&=\sum_{k=0}^{h+1}\sum_{l=0, l\neq h+1}^{p-1}\sum_{j=2}^{p-2}\{pk+1, pl+j\} + \sum_{k=h+2}^{p}\sum_{l=0, l\neq h+1}^{p-1}\sum_{j=2}^{p-2}\{pk-1, pl+j\}\\
&+\sum_{k=0}^{h+1}\sum_{l=0, l\neq h+1}^{p-1}\sum_{j=2}^{p-2}\Big(\{p, pl+j\} + \{-p, pl+j\}\Big) + 2(h+1)\sum_{k=0}^{h+1}\sum_{j=2}^{p-2}\{pk+1, pj\}\\
&+2(h+1)\sum_{k=h+2}^{p}\sum_{j=2}^{p-2}\{pk-1, pj\} + 2(h+2)(h+1)\sum_{j=2}^{p-2}\Big(\{p, pj\} + \{-p, pj\}\Big).
\end{aligned}
$$

Thus

$$
\begin{aligned}
&\sum_{k=0}^{h+1}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,1}, g_{l,j}\} + \sum_{k=0}^{h+1}\sum_{j=2}^{h+1}\{g_{k,1}, g_{h+1,j}\}\\
&=\sum_{k=0}^{h+1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk+1, pl+j\} + \sum_{k=h+2}^{p}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk-1, pl+j\}\\
&+\frac{p+1}{2}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big(\{p, pl+j\} + \{-p, pl+j\}\Big) + p\sum_{k=0}^{h+1}\sum_{j=2}^{p-2}\{pk+1, pj\}\\
&+p\sum_{k=h+2}^{p}\sum_{j=2}^{p-2}\{pk-1, pj\} + \frac{p(p+1)}{2}\sum_{j=2}^{p-2}\Big(\{p, pj\} + \{-p, pj\}\Big).
\end{aligned}
$$

Similarly,

$$\begin{aligned}
&\sum_{k=0}^{h}\sum_{l=0}^{h}\sum_{j=2}^{p-2}\{g_{k,p-1},g_{l,j}\}+\sum_{k=0}^{h}\sum_{j=2}^{h+1}\{g_{k,p-1},g_{h+1,j}\}\\
=&\sum_{k=1}^{h+1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk-1,pl+j\}+\sum_{k=h+2}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk+1,pl+j\}\\
&+\frac{p-1}{2}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big(\{p,pl+j\}+\{-p,pl+j\}\Big)+p\sum_{k=1}^{h+1}\sum_{j=2}^{p-2}\{pk-1,pj\}\\
&+p\sum_{k=h+2}^{p-1}\sum_{j=2}^{p-2}\{pk+1,pj\}+\frac{p(p-1)}{2}\sum_{j=2}^{p-2}\Big(\{p,pj\}+\{-p,pj\}\Big).
\end{aligned}$$

Altogether the expression in the claim is reduced to

$$\begin{aligned}
X:=&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk+1,pl+j\}+\sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\{pk-1,pl+j\}\\
&+p\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big(\{p,pl+j\}+\{-p,pl+j\}\Big)+p\sum_{k=0}^{p-1}\sum_{j=2}^{p-2}\{pk+1,pj\}\\
&+p\sum_{k=1}^{p}\sum_{j=2}^{p-2}\{pk-1,pj\}+p^2\sum_{j=2}^{p-2}\Big(\{p,pj\}+\{-p,pj\}\Big).
\end{aligned}$$

To see this last expression can be reduced to 0 we recall that by definition [17, (5.13.6)]

$$\{a,b\}=\{e_a,e_b\}=[e_a,e_b]+\partial_a(e_b)-\partial_b(e_a),$$

where ∂_a is the derivation defined by $\partial_a(e_0)=0$ and $\partial_a(e_\zeta)=[-[\zeta](e_a),e_\zeta]$ for any p^2th root of unity ζ (see [17, (5.13.4)]). Thus by abuse of notation $[x,y]=[e(x),e(y)]$ we get

$$\begin{aligned}
X=&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big([pk+1,pl+j]-[p(k+l)+j+1,pl+j]\\
&\qquad\qquad+[p(k+l)+j+1,pk+1]\Big) \qquad (42)\\
&+\sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big([pk-1,pl+j]-[p(k+l)+j-1,pl+j]\\
&\qquad\qquad+[p(k+l)+j-1,pk-1]\Big) \qquad (43)\\
&+p\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}\Big([p,pl+j]-[p(l+1)+j,pl+j]+[p(l+1)+j,p]
\end{aligned}$$

$$+[-p, pl+j] - [p(l-1)+j, pl+j] + [p(l-1)+j, -p]\Big) \tag{44}$$

$$+p\sum_{k=0}^{p-1}\sum_{j=2}^{p-2}\Big([pk+1, pj] - [p(j+k)+1, pj] + [p(j+k)+1, pk+1]\Big) \tag{45}$$

$$+p\sum_{k=1}^{p}\sum_{j=2}^{p-2}\Big([pk-1, pj] - [p(j+k)-1, pj] + [p(j+k)-1, pk-1]\Big) \tag{46}$$

$$+p^2\sum_{j=2}^{p-2}\Big([p, pj] - [p(j+1), pj] + [p(j+1), p] + [-p, pj] - [p(j-1), pj] + [p(j-1), -p]\Big). \tag{47}$$

Now by skew-symmetry of Lie bracket

$$\begin{aligned}
&(42)+(43)\\
=&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}[pk+1, pl+j] + \sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}[pk+j, pl+j+1]\\
-&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}\sum_{j=3}^{p-1}[pk+1, pl+j] + \sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=2}^{p-2}[pk-1, pl+j]\\
-&\sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=1}^{p-3}[p(k+l)+j, pl+j+1] + \sum_{k=1}^{p}\sum_{l=0}^{p-1}\sum_{j=1}^{p-3}[pl+j, pk-1]\\
=&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}[pk+1, pl+2] + \sum_{k=0}^{p-1}\sum_{l=0}^{p-1}[pk+p-2, pl+p-1]\\
-&\sum_{k=0}^{p-1}\sum_{l=0}^{p-1}[pk+1, pl+p-1] + \sum_{k=1}^{p}\sum_{l=0}^{p-1}[pk-1, pl+p-2]\\
-&\sum_{k=1}^{p}\sum_{l=0}^{p-1}[pk+1, pl+2] + \sum_{k=1}^{p}\sum_{l=0}^{p-1}[pl+1, pk-1] = 0.
\end{aligned}$$

Similarly we can easily find that (44) = (45) = (46) = (47) = 0. This finishes the proof of the theorem. □

Remark 8.4. The theorem corrects a misprint in the statement of [30, Thm. 2].

In the three cases $(w, N) = (2, 8), (2, 10)$ and $(2, 12)$ we see that $SR(N) > d(w; N) = D(w; N)$. By numerical computation we have

Conjecture 8.5. *We have*

$$d(2, 8) = 9, \quad d(2, 10) = d(2, 12) = 15,$$

and the following relations are the linearly independent non-standard relations: let $L_N(-)=L_N(1,1|-)$ *and* $L_N^{(2)}(-)=L_N(2|-)$*, then*

$$\begin{aligned}37L_8(1,1)=&34L_8^{(2)}(5)+112L_8(3,1)+11L_8(3,0)+37L_8^{(2)}(1)-2L_8(2,6)\\&+3L_8(7,3)-111L_8(5,7)+38L_8(7,7)-8L_8(5,5),\end{aligned}\tag{48}$$

$$\begin{aligned}7L_{10}(5,2)=&72L_{10}^{(2)}(1)+265L_{10}^{(2)}(7)-7L_{10}(2,5)+64L_{10}(9,8)+14L_{10}(5,6)\\&-467L_{10}(4,2)+467L_{10}(8,6)-164L_{10}(9,4)+166L_{10}(7,9)\\&-260L_{10}(8,1)-66L_{10}(3,9)-7L_{10}(6,9)+7L_{10}(6,5).\end{aligned}\tag{49}$$

$$\begin{aligned}L_{12}(8,7)=&5L_{12}^{(2)}(5)+8L_{12}(8,10)-6L_{12}(10,11)-8L_{12}(9,11)+L_{12}(10,9)\\&-15L_{12}(8,1)+5L_{12}(9,10)+5L_{12}(6,1)-L_{12}(1,1)\\&+6L_{12}(8,11)-11L_{12}(6,11)+8L_{12}(8,3)-L_{12}(11,8),\end{aligned}\tag{50}$$

$$\begin{aligned}60L_{12}(8,11)=&38L_{12}(8,7)+348L_{12}(10,11)+502L_{12}(9,11)\\&-492L_{12}(10,9)+600L_{12}(8,1)-552L_{12}(9,10)\\&-154L_{12}(11,10)+20L_{12}(6,1)+261L_{12}(6,11)\\&-502L_{12}(8,3)+221L_{12}(11,8)-319L_{12}(8,10),\end{aligned}\tag{51}$$

$$\begin{aligned}221L_{12}(1,1)=&1854L_{12}(8,10)+562L_{12}(8,7)-1018L_{12}(10,11)\\&-2416L_{12}(9,11)+319L_{12}(10,9)-4270L_{12}(8,1)\\&+2293L_{12}(9,10)+956L_{12}(11,10)+1110L_{12}(6,1)\\&+2416L_{12}(8,11)-3305L_{12}(6,11)+2416L_{12}(8,3).\end{aligned}\tag{52}$$

When N is a non-standard level we find that very often there are non-standard relations among MPVs. For examples, the five relations in Conjecture 8.5 are discovered only through numerical computation. On the other hand, we expect that the standard relations are enough to produce all the linear relations when N *is* standard. In weight two, when N is a prime the answer is confirmed by the next theorem if one assumes a variant of Grothendieck's period conjecture. Computations above provided the primary motivation of this result at the initial stage of this work.

THEOREM 8.6. ([30]) *Let* $p\ge 5$ *be a prime. Then*

$$d(2,p)\le \frac{(5p+7)(p+1)}{24}.$$

If the conjecture in [17, 5.27(c)] *is true then the equality holds and the standard relations in* $\mathcal{MPV}(2,p)$ *imply all the others.*

Proof. See the proof of [30, Thm. 1]. □

It follows from [30, (6)] that the kernel β_p has dimension

$$k(p)=\frac{p^2-1}{24}$$

for all prime $p\ge 5$. From the data in Table 1 we have

Conjecture 8.7. *(a) For all prime $p \geq 5$ kernel β_{p^2} has dimension*

$$k(p^2) = \frac{p(p-1)(p-2)(p-3)}{24}.$$

As a consequence, the upper bound of $d(2,p^2)$ produced by the standard relations is

$$d(2,p^2) \leq \frac{5p^4 - 6p^3 + 19p^2 - 18p + 24}{24}.$$

(b) The standard relations produce all the linear relations and the upper bound in (a) is sharp.

Conjecture 8.8. *(a) For all prime $p \geq 5$ kernel β_{p^3} has dimension*

$$k(p^3) = \frac{p^2(p-1)(p-2)(p-3)(p-4)}{24}.$$

As a consequence, the upper bound of $d(2,p^3)$ produced by the standard relations is

$$d(2,p^3) \leq \frac{5p^6 - 2p^5 - 29p^4 + 74p^3 - 48p^2 + 24}{24}.$$

(b) The standard relations produce all the linear relations and the upper bound in (a) is sharp.

9 Computational results in weight three, four and five

In this last section we briefly discuss our results in weight three, four and five. Since the computational complexity increases exponentially with the weight we cannot do as many cases as we have done in weight two.
Combining the FDS (28), (29), RDS (30)-(35), and the weight one relations (13) and using MAPLE we have verified that $d(3,1) = 1, d(3,2) \leq 3, d(3,3) \leq 8$....

N	1	2	3	4	5	6	7
$SR(3)$	1	3	8	9	22	23	50
$D(3)$	1	3	8	8	27	21	64
$SR(4)$	1	5	16	21	61	69	
$D(4)$	1	5	16	16	81	55	256
$SR(5)$	2	8	32				
$D(5)$	2	8	32	32	243	144	1024
N	8	9	10	11	12	13	
$SR(3)$	38	67	70	157	94	246	
$D(3)$	27	64	56	216	56	343	

Table 2: Upper bounds of $d(w,N)$ by the standard relations and [17, 5.25].

We have done similar computation in other small weight and low level cases and listed the results in Table 2. The values of Deligne and Goncharov's bound $D(w) = D(w,N)$ in Table 2 should be compared with the bound $SR(w) = SR(w,N)$ obtained by the standard relations.
Note that $SR(3,4) = D(3,4) + 1$. By numerical computation using EZface [9] and GiNac [27] we find the following non-standard relation in weight 3:

$$\begin{aligned}5L_4(1,2|2,3) =&46L_4(1,1,1|1,0,0) - 7L_4(1,1,1|2,2,1) - 13L_4(1,1,1|1,1,1)\\&+ 13L_4(1,2|3,1) - L_4(1,1,1|3,2,0) + 25L_4(1,1,1|3,0,0)\\&- 8L_4(1,1,1|1,1,2) + 18L_4(2,1|3,0), \end{aligned}\tag{53}$$

and five non-standard relations in weight 4:

$$\begin{aligned}0 =& - 255608l_1 - 265360l_2 - 219216l_3 - 19306179l_4 - 214008l_5 + 45560l_6\\&- 148296l_7 - 1117280l_8 - 677152l_9 + 86512l_{10} - 239320l_{11} - 50032l_{12}\\&- 121008l_{13} - 96944l_{14} + 202328l_{15} - 1178499l_{16} + 98944l_{17}\\&+ 1565754l_{18} + 23071580l_{19} + 363568l_{20} - 3310177l_{21}, \end{aligned}\tag{54}$$

$$\begin{aligned}0 =&29752l_1 + 23312l_2 + 10960l_3 + 6123413l_4 + 16440l_5 - 12408l_6\\&+ 7144l_7 + 58272l_8 + 86976l_9 - 15952l_{10} + 41144l_{11} + 13552l_{12}\\&+ 29552l_{13} + 9840l_{14} - 36696l_{15} + 375805l_{16} - 41760l_{17}\\&- 477366l_{18} - 7196900l_{19} - 62128l_{20} + 1048983l_{21}, \end{aligned}\tag{55}$$

$$\begin{aligned}0 =&477444l_1 + 431352l_2 + 268168l_3 + 98404710l_4 + 308964l_5 - 233140l_6\\&+ 130028l_7 + 1563872l_8 + 1516032l_9 - 296664l_{10} + 702308l_{11} + 190136l_{12}\\&+ 506440l_{13} + 141592l_{14} - 636468l_{15} + 6027441l_{16} - 701600l_{17}\\&- 7683609l_{18} - 115803282l_{19} - 1063768l_{20} + 16877562l_{21}, \end{aligned}\tag{56}$$

$$\begin{aligned}0 =& - 5976l_1 + 1776l_2 + 8496l_3 - 2132671l_4 + 3176l_5 + 1752l_6\\&+ 3832l_7 + 50976l_8 - 2688l_9 + 2320l_{10} - 10264l_{11} - 5808l_{12}\\&- 6128l_{13} + 2320l_{14} + 8120l_{15} - 132307l_{16} + 13856l_{17}\\&+ 162614l_{18} + 2487604l_{19} + 12720l_{20} - 368485l_{21}, \end{aligned}\tag{57}$$

$$\begin{aligned}0 =& - 474064l_1 - 405248l_2 - 243520l_3 - 54556373l_4 - 283952l_5 + 84368l_6\\&- 170640l_7 - 1033056l_8 - 994784l_9 + 174880l_{10} - 540432l_{11} - 156544l_{12}\\&- 240512l_{13} - 49344l_{14} + 411152l_{15} - 3357683l_{16} + 292256l_{17}\\&+ 4291792l_{18} + 64572648l_{19} + 743136l_{20} - 9470695l_{21}. \end{aligned}\tag{58}$$

where by setting $L = L_4$, $1^4 = \{1\}^4$, ...

$$\begin{aligned}&l_1 = L(1^4|2,1,0,1), && l_2 = L(1^4|2,1^2,0), && l_3 = L(1^4|2,0,3,1),\\&l_4 = L(1^4|2,0^3), && l_5 = L(1^4|1,2,0,3), && l_6 = L(1^4|3^2,0,3),\\&l_7 = L(1^4|3,1,3,2), && l_8 = L(1^4|3,0^3), && l_9 = L(1^4|3,0,1,0),\\&l_{10} = L(1^4|3,0,1^2), && l_{11} = L(2,1^2|0,3,0), && l_{12} = L(3,1|0,3),\\&l_{13} = L(1^4|2,2,3,0), && l_{14} = L(2,1^2|3,1^2), && l_{15} = L(2,1^2|3,0,3),\\&l_{16} = L(1^2,2|2^3), && l_{17} = L(1^4|2,0,1,0), && l_{18} = L(2,1^2|2^2,0),\\&l_{19} = L(1^4|\{2,0\}^2), && l_{20} = L(2^2|3,0), && l_{21} = L(1^4|2^4).\end{aligned}$$

We now can prove this by using the octahedral symmetry of $\mathbb{P}^1-(\{0,\infty\}\cup\boldsymbol{\mu}_4)$ (see Remark 5.3). This idea was suggested to the author by Deligne in a letter dated Feb. 14, 2008.

Theorem 9.1. ([30]) *If the conjecture in* [17, 5.27(c)] *is true then all the linear relations among MPVs of level four and weight three (resp. weight four) are the consequences of the standard relations and the octahedral relation* (53) *(resp. the five octahedral relations* (54)-(58)*).*

Proof. For the proof please see[30, §3]. □

From the available data in Table 2 we can formulate the following conjecture.

Conjecture 9.2. *Suppose the level $N=p$ is a prime ≥ 5. Then*

$$d(3,p)\leq \frac{p^3+4p^2+5p+14}{12}.$$

Moreover, equality holds if standard relations produce all the linear relations.

We formulated this conjecture under the belief that the upper bound of $d(3,p)$ produced by the standard relations should be a polynomial of p of degree 3. Then we find the coefficients by the bounds of $d(3,p)$ for $p=5,7,11,13$ in Table 2.
When $w>2$ it's not too hard to improve the bound of $d(w,p)$ given in [17, 5.25] by the same idea as used in the proof of [17, 5.24] (for example, decrease the bound by $(p^2-1)/24$). But they are often not the best. We conclude our paper with the following conjecture.

Conjecture 9.3. *If N is a standard level then the standard relations always provide the sharp bounds of $d(w,N)$, namely, all linear relations can be derived from the standard ones, if further $N>3$ then the bound $D(w,N)$ in* (36) *by Deligne and Goncharov can be lowered. If N is a non-standard level then the bound $D(w,N)$ is sharp and there exists a positive integer $w_0(N)$ so that at least one non-standard relation exists in $\mathcal{MPV}(w,N)$ for each $w\geq w_0(N)$.*

It is likely that one can take $w_0(4)=w_0(6)=w_0(9)=3$ and $w_0(N)=2$ for all the other non-standard levels N.

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