Formal Computations About Multiple Zeta Values

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Abstract. In this paper, we compute the dimensions of the graded Lie algebra $\mathfrak{dmr}_0$ (introduced by Racinet in [Rac00]) up to a given degree. These results prove that, up to this degree, the Lie algebra $\mathfrak{dmr}_0$ is free over one element in each odd degree greater than or equal to 3, this element being the one introduced by Drinfeld in [Dri90] and belonging to his Lie algebra $\mathfrak{grt}_1$. In particular, this proves, up to the same degree, that the double shuffle and regularization relations imply the associators relations, and that the formal dimension conjecture of Zagier is true.

Keywords: Shuffle Products, Multiple Zeta Values, Zeta Function, Associators, Free Lie Algebras, Quasi-symmetric Functions, Conjecture of Deligne-Drinfeld, Grothendieck-Teichmüller Group.

1 Introduction

The numbers we call Multiple Zeta Values (MZVs, for short) are values at positive integers of the following generalization of Riemann's Zeta function:

$$\zeta(s_1, \ldots, s_r) := \sum_{n_1 > n_2 > \cdots > n_r > 0} 1/n_1^{s_1} n_2^{s_2} \cdots n_r^{s_r} \qquad (1)$$

For such sequences of positive integers, this series will be finite if and only if $s_1 \neq 1$. There has been a big amount of research around these numbers during the past decade, either theoretical or computational, since Zagier's talk at the first ECM [Zag94].

Many combinatorial problems related to quantum algebra become simpler if the base field contains the MZVs. This happens because their full collection is the only explicitly defined solution of some relevant infinite system of equations. This is an obstruction to let the computers work on these problems, since the transcendance properties of the MZVs seem to be out of reach. There are however precise transcendance conjectures about the MZVs. For instance, Zagier conjectured that the dimensions d_n of the $\mathbb{Q}$-vector subspace of $\mathbb{R}$ spanned by the MZVs of weight $n = s_1 + \cdots + s_r$ should satisfy the Fibonacci-like $d_n = d_{n-2} + d_{n-3}$.

In this paper, we will focus on two infinite systems of algebraic relations between the MZVs: the "regularized double shuffle" relations (DMR)[1] and the associators relations. The latter already led to an impressive amount of applications [EK96, BN97, Piu95, Car93, Kon99, Tam], and the former are somewhat simpler. Both are conjecturally equivalent. One of the goals of this paper is to check that the DMR relations imply the associators', up to a given weight. Our method relies on results of the third author [Rac01, Rac02], that allow to perform this task without writing down the relations of the associators. Anyway, let us sketch for completeness some parts of this theory.

Let a and b be two formal non-commuting symbols. In the seminal paper [Dri91], Drinfeld introduced the associators, which he defined as the Lie exponentials Φ built on a, b which satisfy:

$$\Phi(b,a)\Phi(a,b) = 1 \quad \text{(duality, or 2-cycle)} \tag{2}$$
$$e^{\lambda a}\Phi(c,a)e^{\lambda c}\Phi(b,c)e^{\lambda b}\Phi(a,b) = 1 \quad \text{(hexagonal, or 3-cycle),} \tag{3}$$

where c stands for $-a-b$ and λ is a scalar, together with a third equation, called *pentagonal*, or *5-cycle*, which is more complicated. These equations are equivalent to an infinite system of constraints between the coefficients of Φ. Using the monodromy properties of the formal Knizhnik-Zamolodchikov differential equations, Drinfeld built an associator Φ_{KZ} with complex coefficients. Although he proved the existence of rational associators, none has so far been *constructed*. It was later understood that Φ_{KZ} is some kind of non-commutative generating series encoding all the MZVs [LM96, NPH99]. We can therefore understand Drinfeld's equations as a system of relations between them.

Drinfeld also introduced two infinite matrix groups acting on associators, the Grothendieck-Teichmüller group GT_1 and its "graded" version GRT_1. The

[1] This stands for the french "Double mélange et régularisation".

Lie algebra $\mathfrak{grt}_1$ of GRT_1, also known as Ihara's "stable derivation algebra" [Iha92] has also very interesting relationships with the absolute Galois group $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ (see [Iha91] for an excellent review of these topics).

The third author introduced a graded Lie algebra $\mathfrak{dmr}_0$ playing the role of $\mathfrak{grt}_1$ in the DMR setting. In this paper, we prove by computer computation the inclusion of $\mathfrak{dmr}_0$ in $\mathfrak{grt}_1$.[2] This is easily seen to mean that the DMR relations imply the associators relations. For fastening up the computation, we use insights from Drinfeld's conjectural description of $\mathfrak{grt}_1$, which we call Deligne-Drinfeld conjecture for convenience. Indeed, we prove it, with $\mathfrak{grt}_1$ being replaced by $\mathfrak{dmr}_0$. This gives for $\mathfrak{grt}_1$ still one half of the conjecture – the freeness part. The full result about $\mathfrak{dmr}_0$ also proves the counterpart of Zagier's conjecture for formal consequences of the DMR system.

Some related computations were done by the Lille team up to weight 10 [NP00], then 12 [BJOP98]. They computed a Gröbner basis of the DMR system[3] and checked that Zagier's conjecture is true for DMR, up to this weight. The price to pay for the method we use here is that it provides all relations between MZV's deduced from DMR only up to some rational multiple of $\zeta(2)^n$ in weight $2n$.

1.1 Structure of the paper

We first quickly review the first properties of the MZVs and the double shuffle and regularization relations (see Section 2). We then introduce the algebra of formal MZVs and its dual variety DMR (see Section 3). Next, we give the definition of the Lie algebra $\mathfrak{dmr}_0$ and state the main theorem of [Rac02]. We then discuss the conjectural description of Drinfeld's $\mathfrak{grt}_1$ and explain some reductions (see Section 4). Finally, we describe the implementation of the computation in Section 6.

1.2 Acknowledgments

The authors would like to thank Tobias Weingartner and the Department of Computer Science of University of Alberta, Canada, for gracious use of their computing resources.

[2] Here and below, all results are valid up to weight 19.

[3] Seemingly, they use only a subset of DMR. The same argument as in the present article fills the gap.

2 Multiple zeta values and double shuffle relations

Throughout this paper, $\mathbb{K}$ denotes a commutative ring with unit which contains $\mathbb{Q}$, the field of rationals, $\mathbb{K}\langle A\rangle$ denotes the algebra of non commutative polynomials over the set A, and $\mathbb{K}\langle\langle A\rangle\rangle$ denotes the algebra of formal series over A. We will denote by A^* the set of words on A; the empty word will be denoted ϵ.

Finally, the letter S will represent the set of ordered sequences of strictly positive integers (also known as compositions) and S^{cv} the subset of sequences that do not begin with 1.

2.1 First shuffle relations

The first shuffle relations come from some well-known iterated integral representation of MZVs (Multiple Zeta Values) that will not be discussed in this paper (see, *e.g.*, [Gon00]). We will only present how these relations translate in the multiple zeta values context.

2.1.1 The usual shuffle product All the material presented in this paragraph can be found with much more details in [Reu93].

Let X be the alphabet $X = \{x_0, x_1\}$. Let a and b be two elements of X^* written as $a = a_1a'$ and $b = b_1b'$, where a_1 and b_1 belong to X. Then one recursively defines the *shuffle product* of a and b as

$$(a_1a') ⧢ (b_1b') = a_1(a' ⧢ b_1b') + b_1(a_1a' ⧢ b'), \tag{1}$$

with $\epsilon ⧢ x = x ⧢ \epsilon = x$, for every x in X^*.

For example, one can check that

$$x_0x_1 ⧢ x_0x_0x_1 = x_0x_1x_0x_0x_1 + 3x_0x_0x_1x_0x_1 + 6x_0x_0x_0x_1x_1. \tag{2}$$

It is known that the shuffle product endows $\mathbb{K}\langle X\rangle$ with a free commutative algebra structure.

We will have later to consider two subalgebras of $\mathbb{K}\langle X\rangle$. The first one is the algebra $\mathbb{K}(X^c)$ spanned by X^c, the set of words in X that do not end with an x_0 (it is closed since the shuffle of two words that do not end with an x_0 is a linear combination of such words). The second one is the algebra $\mathbb{K}(X^{cv})$, where X^{cv} is the set of words in X that do not end with an x_0 and do not begin with an x_1.

One can endow the usual concatenation algebra $(\mathbb{K}\langle X\rangle, \cdot)$ with a Hopf algebra structure, the coproduct $\Delta\colon \mathbb{K}\langle X\rangle \to \mathbb{K}\langle X\rangle \otimes \mathbb{K}\langle X\rangle$ being given as an algebra morphism by

$$\Delta x_i = 1 \otimes x_i + x_i \otimes 1, \quad i \in \{0,1\}.$$

There is a well-known duality between Δ and $\sqcup\!\sqcup$ that will be used implicitly in Section 3.

2.1.2 Connection with the Multiple Zeta Values Let us begin with some notation. If x belongs to X^c, one can write x as

$$x = x_0^{s_1-1}x_1x_0^{s_2-1}x_1 \cdots x_0^{s_r-1}x_1, \tag{3}$$

where $\mathbf{s} = (s_1, \ldots, s_r)$ is an element of S. So there exists a natural bijection between X^c and S: the word x written in Equation (3) is associated with the sequence $\mathbf{s}$. Notice that this correspondence provides a bijection between X^{cv} and S^{cv}, as well.

Thanks to this bijection, one can define $\mathbf{s} \sqcup\!\sqcup \mathbf{s}'$ with $\mathbf{s}$ and $\mathbf{s}'$ in S, as the shuffle of the two corresponding elements of X^c, expressed as a formal sum of elements of S.

With this notation, one can now state the *shuffle relations of the first kind* as

$$\forall \mathbf{s}, \mathbf{s}' \in S^{cv}, \; \zeta(\mathbf{s})\zeta(\mathbf{s}') = \zeta(\mathbf{s} \sqcup\!\sqcup \mathbf{s}'). \tag{4}$$

where ζ is extented by linearity to formal sums.

For example, if one considers $\mathbf{s} = (2)$ and $\mathbf{s}' = (3)$, the two equations (2) and (4) lead to

$$\zeta(2)\zeta(3) = \zeta(2,3) + 3\zeta(3,2) + 6\zeta(4,1). \tag{5}$$

Remark 2.1 For $\mathbf{s} = (s_1, \ldots, s_r)$, one defines the *weight* $w(\mathbf{s})$ of $\mathbf{s}$ as $\sum s_i$. One can then easily see that the usual shuffle product is a homogeneous operation with respect to the weight on sequences. Notice that this weight exactly is the total degree of the corresponding word in X^*, whereas the length r is the partial degree in x_1.

2.2 The second shuffle relations

The second shuffle relations can be understood as the product of monomial quasi-symmetric functions, as defined in [Ges84] and extensively studied in [GKL+95, MR95]. Indeed, the MZVs appear as special values of these functions.

2.2.1 The second shuffle product For notation safety, we shall (tautologically) replace finite sequences by words built on an infinite alphabet of non-commuting letters $Y = \{y_1, y_2, \ldots\}$.

For any words $u, v \in Y^*$ and positive integers p, q, the product $*$ is given by the following recursive formula:

$$\begin{gathered}(y_p u) * (y_q v) = (u * y_q v) + y_q(y_p u * v) + (y_{p+q})(u * v),\\ \epsilon * u = u * \epsilon = u,\end{gathered} \tag{6}$$

where u and v are any words in Y^* and p, q are positive integers. For example, we have

$$y_2 * y_3 = y_2 y_3 + y_3 y_2 + y_5. \tag{7}$$

Remark 2.2 Moreover, one can endow the *concatenation* algebra $(\mathbb{K}\langle Y\rangle, \cdot)$ with a bialgebra structure with coproduct Δ_* defined as

$$\forall n \in \mathbb{N},\ \Delta_*(y_n) = \sum_{k+l=n} y_k \otimes y_l, \quad \text{with } y_0{:=}1 \tag{8}$$

It is then known that the coproduct is dual to the product $*$ (see [MR95]).

2.2.2 Connection with the Multiple Zeta Values As we mentionned before, the MZVs are specializations of quasi-symmetric functions and thus inherit the following property, as was extensively studied in [Hof95, Hof97]:

$$\forall \mathbf{s}, \mathbf{s}' \in S^{cv},\ \zeta(\mathbf{s})\zeta(\mathbf{s}') = \zeta(\mathbf{s} * \mathbf{s}'), \tag{9}$$

where the product $*$ is interpreted on sequences.

This can also be proved by direct induction on the definition in Formula (1).

In the situation of the example (5), we now have, by Equations (7) and (9):

$$\zeta(2)\zeta(3) = \zeta(2,3) + \zeta(3,2) + \zeta(5). \tag{10}$$

Remark 2.3 As in the case of the first shuffle product, one can easily see that the second shuffle product is a homogeneous operation for the weight on sequences.

These examples also illustrate that the similitudes in the combinatorial descriptions of the two kinds of shuffle relations do not prevent them from being quite incompatible. Actually, the evidence of existence of the MZVs is the only known proof of the fact that the two shuffle relations don't contradict each other. The same remark holds for associators.[4]

[4]For associators, there is another such evidence, coming from their ℓ-adic counterparts.

2.3 Regularization process

It is convenient to give sense to divergent MZVs (*e.g.* $\zeta(1)$) with respect to each shuffle product, so that either Equation (4) or Equation (9) still holds. The main reason is that it would allow us to define generating series of *all* MZVs that would be by construction group-like elements in the Hopf algebras previously defined and thus would allow us to use powerful algebraic tools. For complete explanations about this part, see, *e.g.*, [Rac00, Hof97, NP00]. The process that associates a finite value with each divergent MZV is called the *regularization process.*

In the sequel, we denote by $(\Phi|w)$, where w belongs to A^* and $\Phi \in \mathbb{K}\langle\langle A\rangle\rangle$, the coefficient of w in Φ. We extend this definition by linearity on the right to any element of $\mathbb{K}\langle A\rangle$.

2.3.1 Regularization of the usual shuffle product

Proposition 2.4 ([NPH98]) *There exists a unique series $\Phi_{\sqcup\!\sqcup}$ in $\mathbb{R}\langle\langle X\rangle\rangle$ satisfying*

$$\Delta(\Phi_{\sqcup\!\sqcup}) = \Phi_{\sqcup\!\sqcup} \otimes \Phi_{\sqcup\!\sqcup} \tag{11}$$

such that the coefficient of x_0 and x_1 are zero and the coefficient of every element x of X^{cv} is equal to $\zeta(\mathbf{s})$ where $\mathbf{s}$ is the element of S associated with x.

This proposition allows us to compute $(\Phi_{\sqcup\!\sqcup}|w)$ for a given word w, even if it begins with x_1 and/or ends with x_0 for $\Phi_{\sqcup\!\sqcup}$ being a Lie exponential is equivalent to the relation

$$\forall u, v \in X^*, (\Phi_{\sqcup\!\sqcup}|(u \sqcup\!\sqcup v)) = (\Phi_{\sqcup\!\sqcup}|u)(\Phi_{\sqcup\!\sqcup}|v), \tag{12}$$

and is also equivalent to $\Phi_{\sqcup\!\sqcup}$ being a group-like element, that is

$$\Delta\Phi_{\sqcup\!\sqcup} = \Phi_{\sqcup\!\sqcup} \otimes \Phi_{\sqcup\!\sqcup}. \tag{13}$$

For example, one computes that

$$(\Phi_{\sqcup\!\sqcup}|x_1x_1) = 0, \tag{14}$$

since $x_1 \sqcup\!\sqcup x_1 = 2x_1x_1$. Let us mention that there exists a simple formula given by Cartier (see [Car00]), to directly compute each coefficient of $\Phi_{\sqcup\!\sqcup}$ using the Taylor expansion.

It is now well known that $\Phi_{\sqcup\!\sqcup}$ and Drinfeld's Φ_{KZ} series are equal, if one identifies a with x_0 and b with $-x_1$.

2.3.2 Regularization of the second shuffle product

Proposition 2.5 *There exists a unique series Φ_* in $\mathbb{R}\langle\langle Y\rangle\rangle$ satisfying*

$$\Delta_*(\Phi_*) = \Phi_* \otimes \Phi_* \tag{15}$$

such that the coefficient of y_1 is zero and the coefficient of an element y of Y^{cv} is equal to $\zeta(\mathbf{s})$ where $\mathbf{s}$ is the element of S associated with y.

This last proposition allows us to compute $(\Phi_*|w)$ for a given word w, even if it begins with y_1 for Φ_* being a group-like element is equivalent to the relation

$$\forall u, v \in Y^*, (\Phi_*|(u * v)) = (\Phi_*|u)(\Phi_*|v). \tag{16}$$

For example, one computes that

$$(\Phi_*|y_1y_1) = -\frac{1}{2}(\Phi_*|y_2) = -\frac{\pi^2}{12}, \tag{17}$$

since $y_1 * y_1 = 2y_1y_1 + y_2$. Again, let us mention that there exists a simple formula to directly compute each coefficient of Φ_* using the Taylor expansion that was given by Cartier (see [Car00]).

Notice that both regularizations do not give the same result for $(1,1)$ (see Equations 14 and 17). Still, some comparison is possible. This is precisely what the last relation (see Proposition 2.6) provides.

2.3.3 Comparison between both regularizations The third system of relations between MZVs can be expressed as a comparison formula between the series $\Phi_{\sqcup\!\sqcup}$ and Φ_* (see, *e.g.*, [Rac02] for more details, including historical remarks):

Proposition 2.6 *The series $\Phi_{\sqcup\!\sqcup}$ and Φ_* are deduced one from the other by the equation*

$$\Phi_* = \exp\left(\sum_{n\geqslant 2} \frac{(-1)^{n-1}}{n}\zeta(n)y_1^n\right)\Pi_Y(\Phi_{\sqcup\!\sqcup}), \tag{18}$$

where Π_Y stands for the linear projection from $\mathbb{R}\langle\langle X\rangle\rangle$ to $\mathbb{R}\langle\langle Y\rangle\rangle$ that sends each word ending with x_0 to 0 and each $x = x_0^{s_1-1}x_1\cdots x_0^{s_r-1}x_1$ to $y_{s_1}\cdots y_{s_r}$.

The first new relation arising from this proposition is

$$\zeta(3) = \zeta(2,1), \tag{19}$$

which dates back to Euler.

Indeed, one can easily check that the coefficient of y_2y_1 on the left-hand side of Equation (18) is $2\zeta(2,1)$, whereas its coefficient on its right-hand side is $\zeta(3)+\zeta(2,1)$.

Let us notice that this third system of relations implies the Hoffman system of relations (see [Hof97, Rac00]).

Remark 2.7 As in the case of the first and the second shuffle product, one can see that the relations summarized by Equation (18) are homogeneous for the weight on sequences. This compatibility of both shuffle products and regularization relations with the weight enables us to study the relations between MZVs weight by weight.

3 Formal MZVs

It is a conjecture that the double shuffle and regularization relations generate all possible algebraic relations with rational coefficients between the MZVs. This conjecture is far out of reach at the present time: it would imply[5] for example the algebraic independence of the $\zeta(2n+1)_{n\geqslant 0}$. Nevertheless, this conjecture suggests to focus on the *formal* consequences of the three above relations.

3.1 The dual variety

One natural way to address this problem would be to consider the algebra PZF of "formal MZVs", *i.e.*, algebra of unknowns $\overline{\zeta}(s)_{s\in S}$ satisfying relations (4), (9), and (18). For many reasons, the most obvious being the compact form that our three relations take on generating series, we shall rather work with the following dual object.

Definition 3.1 For any commutative ring $\mathbb{K}$, such that $\mathbb{Q}\subset\mathbb{K}$, let $\mathsf{DMR}_\lambda(\mathbb{K})$ be the set of elements Φ of $\mathbb{K}\langle\langle X\rangle\rangle$ such that

$$
\begin{aligned}
(\Phi|1) &= 1 &(1)\\
(\Phi|x_0) &= (\Phi|x_1)=0 &(2)\\
(\Phi|x_0x_1) &= \lambda &(3)\\
\Delta\Phi &= \Phi\ \widehat{\underset{\mathbb{K}}{\otimes}}\ \Phi &(4)\\
\Delta_*\Phi_* &= \Phi_*\ \widehat{\underset{\mathbb{K}}{\otimes}}\ \Phi_*, &(5)
\end{aligned}
$$

[5] This is actually an easy consequence of Theorem 3.4 below.

where

$$\Phi_* := \exp\left(\sum_{n\geqslant 2} \frac{(-1)^{n-1}}{n} (\Pi_Y(\Phi)|y_n) y_1^n\right) \Pi_Y(\Phi) \tag{6}$$

The results of the previous sections now read: $\Phi_ш \in \mathsf{DMR}_{\zeta(2)}(\mathbb{R})$. The relevance of this definition to our problem is due to the following easy fact:

Proposition 3.1 *There is a natural bijection between* $\mathsf{DMR}_\lambda(\mathbb{K})$ *and the set of algebra homomorphisms from* PZF *to* $\mathbb{K}$ *sending* $\overline{\zeta}(2)$ *to* λ.

Here "natural" means that it is compatible with maps induced on both sides by algebra morphisms $\mathbb{K} \to \mathbb{K}'$. In other words, $\mathsf{DMR}_\lambda(\mathbb{K})$ is the set of all generating series encoding collections of elements of $\mathbb{K}$ satisfying our three relations, λ playing the role of $\zeta(2)$. By general abstract considerations (Yoneda's Lemma), it is equivalent to study the functor $\mathbb{K} \mapsto \mathsf{DMR}(\mathbb{K})$ in place of PZF.

This change of perspective also makes the comparison with Drinfeld associators easier to perform.

3.2 The Lie algebra

Many properties of DMR can be reduced to the tangent space $\mathfrak{dmr}_0$ at 1 of DMR_0, as it follows from Theorem 3.4 below. Informally speaking, to get the defining equations of this tangent space, one only needs to linearize equations (1)–(6). Here is a direct definition:

Definition 3.2 Let $\mathfrak{dmr}(\mathbb{K})$ be the set of elements ψ of $\mathbb{K}\langle\langle X\rangle\rangle$ such that

$$\begin{aligned} (\psi|1) &= 1 && (7)\\ (\psi|x_0) &= (\psi|x_1) = 0 && (8)\\ \Delta\psi &= \psi\otimes 1 + 1\otimes\psi && (9)\\ \Delta_*\psi_* &= \psi_*\otimes 1 + 1\otimes\psi_*, && (10) \end{aligned}$$

where

$$\psi_* := \Pi_Y(\psi) + \sum_{n\geqslant 2} \frac{(-1)^{n-1}}{n} (\Pi_Y(\psi)|y_n) y_1^n \tag{11}$$

We denote by $\mathfrak{dmr}_0(\mathbb{K})$ the subset of $\mathfrak{dmr}(\mathbb{K})$ of elements ψ such that $(\psi|x_0x_1) = 0$.

Remark 3.3 Notice that all spaces $\mathfrak{dmr}_0(\mathbb{K})$ can be reduced to $\mathfrak{dmr}_0(\mathbb{Q})$ (or $\mathfrak{dmr}_0$, for short) since $\mathfrak{dmr}_0(\mathbb{K}) = \mathfrak{dmr}_0 \otimes \mathbb{K}$, by linearity and homogeneity of the above equations.

The definition of the tangent spaces find its use in the next theorem.

Theorem 3.4 ([Rac01, Rac02]) *Let G and H be elements of* $\mathsf{DMR}_\lambda(\mathbb{K})$. *There exists a unique ψ in $\mathfrak{dmr}_0(\mathbb{K})$ such that* $\exp(s_\psi)G = H$, *where s_ψ is the sum of the right multiplication by ψ with the derivation D_ψ sending x_0 to $[\psi, x_0]$ and x_1 to 0.*

For any $\lambda \in \mathbb{Q}$, the set $\mathsf{DMR}_\lambda(\mathbb{Q})$ is not empty.

Ihara's bracket, $<\psi_1, \psi_2> \ := s_{\psi_1}(\psi_2) - s_{\psi_2}(\psi_1)$ endows $\mathfrak{dmr}_0$ with a Lie algebra structure.

We will explain in detail in Section 4 how to use this theorem to prove that the regularized double shuffle relations imply a given system of relations. Our main example being the system related to the associators of Drinfeld, we shall first recall some of their properties.

4 Some reductions

4.1 Associators and double shuffles

As we mentionned in the introduction, one aim of this paper is to compare the systems of relations coming from the double shuffle and from the associators. We are going to prove that, up to a certain weight, the DMR relations imply the associators relations.

Let $\mathsf{Ass}_\lambda(\mathbb{K})$ denote the set of associators with parameter λ in Equation (3) and with coefficients in $\mathbb{K}$. Let $\mathfrak{grt}_1$ be the tangent space of Ass_0 at 1. Forgetting the weight restriction, our aim restates as proving the inclusion of $\mathsf{DMR}_\lambda(\mathbb{K})$ in $\mathsf{Ass}_\lambda(\mathbb{K})$, for all $\mathbb{K}$ and $\lambda \in \mathbb{K}$.

Actually, Theorem 3.4 was inspired by Drinfeld's results.

Theorem 4.1 (Drinfeld [Dri91], props. 5.5 & 5.9) *Fix $\lambda \in \mathbb{K}$ and let G and H be elements of $\mathsf{Ass}_\lambda(\mathbb{K})$. There is a unique $\psi \in \mathfrak{grt}_1(\mathbb{K})$ such that $\exp(s_\psi)G = H$. Rational associators do exist,* i.e., $\mathsf{Ass}_1(\mathbb{Q}) \neq \varnothing$.

Another common feature of Ass and DMR is the homogeneity of their defining equations. This can be stated as follows: let $[\mu]\Phi$ denote the series deduced from Φ by multiplication of the homogeneous component of weight n by μ^n. Then $\Phi \in \mathsf{Ass}_\lambda(\mathbb{K})$ implies $[\mu]\Phi \in \mathsf{Ass}_{\lambda\mu}(\mathbb{K})$ while $\Phi \in \mathsf{DMR}_\lambda(\mathbb{K})$ implies $[\mu]\Phi \in \mathsf{DMR}_{\lambda\mu^2}(\mathbb{K})$, because the weight of x_0x_1 is 2.

Now, thanks to Theorems 3.4 and 4.1, the comparison of DMR and Ass boils down to the Lie algebras $\mathfrak{dmr}_0$ and $\mathfrak{grt}_1$: let us assume for instance we have the inclusion $\mathfrak{dmr}_0 \subset \mathfrak{grt}_1$. Recall that $\Phi_{⧢}$ belongs to *both* $\mathsf{DMR}_{\zeta(2)}(\mathbb{C})$ and $\mathsf{Ass}_{i\pi}(\mathbb{C})$. Applying $[1/i\pi]$, we thus get a common element of $\mathsf{DMR}_{-1/6}(\mathbb{C})$

and $\mathsf{Ass}_1(\mathbb{C})$. Using both theorems and the Lie algebra inclusion, we get the inclusion of $\mathsf{DMR}_{-1/6}(\mathbb{C})$ in $\mathsf{Ass}_1(\mathbb{C})$, whence in particular of $\mathsf{DMR}_{-1/6}(\mathbb{Q})$ in $\mathsf{Ass}_1(\mathbb{Q})$. Now let Ψ belong to $\mathsf{DMR}_{-1/6}(\mathbb{Q})$. For any $\lambda \in \mathbb{K}$, we thus have a common element $[\lambda]\Psi$ in $\mathsf{DMR}_{-\lambda^2/6}(\mathbb{K})$ and $\mathsf{Ass}_\lambda(\mathbb{K})$. Another use of both theorems completes the task:

$$\forall \mathbb{K},\ \forall \lambda \in \mathbb{K},\ \mathsf{DMR}_{\frac{-\lambda^2}{6}}(\mathbb{K}) \text{ is included in } \mathsf{Ass}_\lambda(\mathbb{K}). \tag{1}$$

If we assume our inclusion up to some weight, the obvious homogeneity properties of the s_ψ's ensure that this implication still holds up to the given weight.

The same argument will obviously work for any couple of systems of $\mathbb{Q}$-algebraic relations between the MZVs, provided they satisfy adapted versions of Theorems 3.4 and 4.1, if one already has the inclusion at the Lie algebra level. This way, one obtains that the "motivic" relations (see [DG]) imply both DMR and the associators' relations, even though we cannot write them down explicitly. It is enough to know the relevant Lie algebra, which happens to be generated by the special elements we shall now introduce.

4.2 Drinfeld's indecomposables

In the last page of [Dri91], Drinfeld relates the following question to conjectures stated by Deligne:

Question 4.1 *Is $\mathfrak{grt}_1$ free as a Lie algebra, with exactly one homogeneous generator of each odd weight different from 1?*

Moreover, he gave a very simple construction of indecomposable elements of $\mathfrak{grt}_1(\mathbb{C})$ with the right weights. Their definition reads as follows: it's not hard to show the equality of $\mathsf{Ass}_{-\lambda}(\mathbb{K})$ and $\mathsf{Ass}_1(\mathbb{K})$. There is therefore an element ψ of $\mathfrak{grt}_1(\mathbb{C})$ such that $\exp(s_\psi)$ maps Φ_{KZ} to $[-1]\Phi_{\mathrm{KZ}}$. Define ψ_n to be the weight n part of ψ. It is non zero if n is odd and at least 3. In that case, the coefficient of $y_n = x_0^n x_1$ in ψ_n is $\zeta(n)$, up to a nonzero rational. This, together with the indecomposability of ψ_n's, follows from the obvious homogeneity of the map $(u,v) \mapsto s_u(v)$ with respect to the partial degrees in x_0 and x_1.

As a direct consequence of Theorem 3.4, these elements belong as well to $\mathfrak{dmr}_0(\mathbb{C})$. As the rank of a linear system is invariant under field extensions, we have as well a collection $(\sigma_{2n+1})_{n\geqslant 0}$ of elements of $\mathfrak{dmr}_0(\mathbb{Q}) \cap \mathfrak{grt}_1(\mathbb{Q})$ in which $x_0^{2n}x_1$ appears with coefficient 1. In particular, the freeness part of the question of Drinfeld can be asserted as well in $\mathfrak{dmr}_0$, while it would be sufficient to prove that $\mathfrak{dmr}_0$ is generated by the collection of the σ_{2n+1} to get the inclusion of $\mathfrak{dmr}_0$ in $\mathfrak{grt}_1$.

5 Experimental protocol

Following those ideas, we first check that the dimension of $\mathfrak{dmr}_0$ is smaller than the dimension of a free algebra with one generator in each component of odd weight greater than or equal to 3. This part is done by Gaussian pivot over huge matrices.

We then get a set of elements that span $\mathfrak{dmr}_0$. In each odd weight, we select one element of this set, in which $x_0^{2n}x_1$ appears with non-zero coefficient and call it τ_{2n+1}. It then remains to check that these elements generate a free algebra up to the given weight.

We detail these two parts with some technical improvements in the next two subsections.

5.1 Computation of an upper bound of $\mathrm{Dim}(\mathfrak{dmr}_0)$

We first present the algorithm used to compute an upper bound of $\mathrm{Dim}(\mathfrak{dmr}_0)$ and next justify it. Since we are only interested in the computation of an upper bound, we made the critical computations with coefficients in some finite field $\mathbb{F}_p$ instead of $\mathbb{Q}$; indeed, this can only increase the value of the upper bound. This does not change the algorithm and allows us to justify it in a more pleasant way.

Algorithm .
INPUT: an integer n.
OUTPUT: a basis of a vector space V_n.

- Step 1. Consider the set of all Lyndon words of X^n and compute the set of standard bracketings of these elements.
- Step 2. Apply the linear map $f \mapsto f_*$, defined by
$$f_* = \Pi_Y(f) + \frac{(-1)^{n-1}}{n}(f|x_0^{n-1}x_1)$$
to the elements obtained in Step 1 and expand the result in the basis of words in Y^*.
- Step 3. Compute the kernel of the operator $\partial_{y_1}^*$ defined by
$$(\partial_{y_1}^*(\psi)|w) = (\psi|y_1 * w), \quad \text{for all } w \in Y^*,$$
on the elements obtained in Step 2.
- Step 4. The algorithm finishes and outputs the kernel.

Remark 5.1 To compute an upper bound of $\mathrm{Dim}(\mathfrak{dmr}_0)$, we have to take into account the relations of double shuffle and regularization. In our algorithm, we introduced these relations in a precise order.

- We first consider the relations coming from the usual shuffle. Let us remind that Equation (9) just means that ψ is a Lie polynomial. So we can start from a basis of the free Lie algebra on X, for instance the Lyndon basis built with the bracketed Lyndon words (see [Reu93] for the definitions). It is Step 1 of our algorithm.
- Step 2 takes into account the relation coming from the regularization process.
- About Step 3, let us first remark that the kernel of $\partial_{y_1}^*$ contains the set of all elements satisfying Equation (10) and whose y_1 coefficient is 0. So the vector space V_n necessarily contains the weight n part of $\mathfrak{dmr}_0$ and its dimension gives the required upper bound.

Remark 5.2 All the computations of the kernels were done by a Gaussian pivot, the last pivots being completely paralel, since the memory of the computers were much smaller than the size of the considered matrices.

5.2 Brackets of τs: lower bound

In the last subsection, we only obtained an upper bound and not the dimension of $\mathfrak{dmr}_0$ in weight n. For each odd n, let us define τ_n as an element of V_n with non-zero coefficient in y_n. We checked by computation on words of small length that the τ_k are free for the Ihara bracket up to weight 19.

If one assumes that the τ_k with $k < n$ indeed are elements of $\mathfrak{dmr}_0$, since σ_n is an indecomposable element of $\mathfrak{dmr}_0$ of weight n, the brackets of the τ_k and σ_n build up a basis of the weight n part of $\mathfrak{dmr}_0$. This gives us the required lower bound for the dimension of the weight n part of $\mathfrak{dmr}_0$. In particular, this proves that τ_n belongs to $\mathfrak{dmr}_0$.

All these remarks prove that, up to weight 19, $\mathfrak{dmr}_0$ is freely generated by one element in each odd degree greater than or equal to 3. It also proves that, up to the same order, $\mathfrak{dmr}_0$ is included in $\mathfrak{grt}_1$.

6 Experimental results

The rank computations were performed on various computers. On a Pentium III 800, the computation for $d = 18$ took less than 4 hours (see Table 1).

The computation for weight 19 was done on an UltraSparc with 4 processors, lent by the university of Alberta, and took about the same time, thanks to a parallelized algorithm. The corresponding memory usage was 700 MB.

The computation for weight 20 should run in less than a day. Unfortunately, some memory problems arise: the matrix is larger than 4 GB. We could fix this by changing our implementation. Switching to a 64-bit system would be a quick, yet unsatisfying solution.

Weight	Dimension of $\mathfrak{dmr}_0$	Time
5	1	
6	0	
7	1	
8	1	
9	1	
10	1	
11	2	
12	2	
13	3	
14	3	
15	4	0h04
16	5	0h15
17	7	1h
18	8	3h30
19	11	

Table 1. Dimension and execution time of our algorithm on a Pentium III

7 Conclusion

In this paper, we proved that up to weight 19, $\mathfrak{dmr}_0$ is freely generated by one element in each odd degree greater than or equal to 3. We also obtained the inclusion $\mathfrak{dmr}_0 \subset \mathfrak{grt}_1$ which in turn means that the system of relations between MZVs coming from the associators is implied by the regularized double-shuffle relations.

We also found a surprising experimental result:

Conjecture 7.1 *The set $\mathfrak{dmr}$ exactly is the set of Lie polynomials ψ such that $\partial^*_{y_1}(\psi) = 0$.*

Let us finally mention, as perspectives, that similar computations can be done about the Lie algebra $\mathfrak{dmrd}_0(\mu_n)$ associated with the more general case of values of multiple polylogarithms at the nth roots of unity.

8 *

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