Steps Towards a Canonical Rational Associator

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Introduction

This thesis aims to discuss and expand upon a collection of interelated problems in number theory, all tying to the theory of multiple zeta values and Drinfel'd associators. Multiple zeta values provide a generalisation of the Riemann zeta function to multiple variables. Where questions of algebraic independence of values of the Riemann zeta function at integer values seem intractable, multiple zeta values have a rich algebraic structure. One interesting question in modern number theory is to describe explicitly this structure, giving all relations among multiple zeta values and describing their Hilbert Poincaré series.

There are several equations describing relations among multiple zeta values, conjecturally describing all relations. The most general of these are Drinfel'd's *associator* equations: functional equations among power series in two non-commuting variables, with solution given by the generating series for multiple zeta values [13]. This adds an extra layer of interest to the study of multiple zeta values: it is known that there is a solution to the associator equations with rational coefficients. Knowing such an object explicitly would be an extremely powerful computational tool: it has applications in the theory of knot invariants [2], the construction of quasitriangular quasi-Hopf algebras, along with providing a tool for decomposition of multiple zeta values into a given basis [4]. As this would give a tool to describe all relations among multiple zeta values explicitly, we make this our end goal: finding a rational associator, using multiple zeta values as a model for the coefficients.

However, solving the associator equations directly proves quite challenging, so we turn to the second set of equations describing relations among multiple zeta values: the double shuffle equations. Arising naturally from the definition of multiple zeta values, these equations are much simpler, and are implied by the associator equations [16]. Conjecturally, they describe all relations among multiple zeta values, and are equivalent to the associator equations. Furthermore, they can easily be considered modulo products, or certain filtrations, allowing us to find relations among "graded" multiple zeta values, which can hopefully be lifted to true relations, reducing the problem of finding rational solutions to the double shuffle equations to that of finding rational solutions modulo products, or a filtration. Indeed, one can reduce many problems about the dimension of the vector space spanned by multiple zeta values to problems about these simplified spaces [5].

In solving these problems, we gain an additional geometric structure: multiple zeta values and the associator equations can by found in the geometry of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. By exploiting this geometric origin, we can produce a motivic Galois group with an action on multiple zeta values, preserving relations. Thus, this Galois group has an action on solutions to the associator and double shuffle equations, which we can exploit in order to attempt to find rational solutions, or to bound the dimension of certain spaces.

This is an incredibly rich and multifaceted problem, and as such, we must summarise it as best we can. The structure of this thesis will be as follows: In section one, we will condense the necessary background material. We first introduce multiple zeta values and their combinatorics, as these play a vital role in describing the object of interest: Drinfel'd associators. These formal power series satisfy certain equations and are used in the construction of quasitriangular quasi-Hopf algebras. However, they are quite mysterious: only 3 examples are known explicitly, and all arise from other areas of mathematics, such as conformal field theory and knot theory. Thus, instead of studying associators directly, we study the Lie group DMR_0 of solutions to the double shuffle equations, allowing us to use the machinery of the motivic Galois group and its ties to $\mathbb{P}^1 \setminus \{0, 1, \infty\}$.

In section two, we consider the Lie algebra $\mathfrak{dmr}_0$ associated to DMR_0, and the equations describing it: the double shuffle equations modulo products. This Lie algebra contains a Lie algebra called the *motivic* Lie algebra, which contains Lie algebraic analogues of associators. It is a free Lie algebra with generators in every odd degree greater than 1, which act on the space of associators, allowing us to produce infinitely many rational associators given one. However, these generators do not have canonical representations, so we discuss methods used to make them canonical: a Gram-Schmidt procedure using inner products, an approach using "polar" solutions, etc. We also consider the linearised double shuffle equations, which describe elements of the associated graded of the motivic Lie algebra, with respect to the depth filtration.

In section three, we introduce some of Brown's motivic machinery: defining motivic multiple zeta values and the motivic coaction. This coaction preserves a filtration - the block filtration - of multiple zeta values, arising from a decomposition due to Charlton, so we expect calculation of the coaction to be simplified in the associated graded. With this in mind, we introduce block graded multiple zeta values, discuss some low weight relations among them and extend the definitions to divergent multiple zeta values. We also compute the coproduct on block graded multiple zeta values modulo $\zeta^{\mathfrak{m}}(2)$, and consider the block graded dual product.

Finally, in section four, we present a slightly eclectic selection of material. We consider possible approaches to deriving the duality relation among multiple zeta values, which arises naturally from the geometry of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, from the double shuffle equations. We also consider the double shuffle equations modulo primes, showing that an integer associator cannot exist and giving hints as to the complexity of coefficients of a rational associator. We expand on a recurring connection between the double shuffle equations and modular forms, before finally briefly acknowledging the analytic structures of multiple zeta functions and how we might exploit this to solve the problem of finding a rational associator.

1 Drinfel'd Associators and the Geometry of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$

1.1 Multiple zeta values and iterated integrals

The field of study surrounding multiple zeta values is deep, wide and sprawling. One cannot hope to give a comprehensive survey of the current state of affairs within the confines of this thesis, and thus we limit ourselves to a brief overview of the bare necessities. For further details, the author recommends [20] or [31] for a more expository recap.

Definition 1.1. For a sequence of integers $(s_1, \ldots, s_r)$ with $s_i \geq 1$ and $s_r \geq 2$, we define the corresponding multiple zeta value by

$$\zeta(s_1, \ldots, s_r) := \sum_{0<n_1<n_2<\ldots<n_r} \frac{1}{n_1^{s_1} n_2^{s_2} \ldots n_r^{s_r}}$$

To a multiple zeta value (often abbreviated MZV), we can associate two quantities: *weight* and *depth*. The weight of $\zeta(s_1, \ldots, s_r)$ is defined to be $s_1 + s_2 + \cdots + s_r$, and the depth is defined to be r

Let $\mathcal{Z}$ be the $\mathbb{Q}$-vector space spanned by multiple zeta values. We can endow this with the structure of an algebra using the *stuffle* relations among MZVs, arising from splitting the summation obtained in the product.

Example 1.2.

$$\begin{aligned} \zeta(2)\zeta(3) &= \sum_{m\geq 1} \sum_{n \geq 1} \frac{1}{m^2 n^3} \\ &= \sum_{m<n\leq 1} \frac{1}{m^2 n^3} + \sum_{n<m\leq 1} \frac{1}{m^2 n^3} + \sum_{n\geq 1} \frac{1}{n^5} \\ &= \zeta(2,3) + \zeta(3,2) + \zeta(5) \end{aligned}$$

Generalising this example, we see that any product of multiple zeta values lies in $\mathcal{Z}$. We make this precise as follows

Definition 1.3. Denote a sequence of positive integers $(i_1, \ldots, i_k)$ by the product $z_{i_1} z_{i_2} \ldots z_{i_k}$ in noncommuting formal variables $z_1, z_2, \ldots$. Denote the empty sequence by 1. Given two sequences of integers, $z_{i_1} \ldots z_{i_r}$ and $z_{j_1} \ldots z_{j_q}$, we recursively define their stuffle product as the formal sum obtained from

$$\begin{aligned} 1 \star z_{i_1} \ldots z_{i_r} &= z_{i_1} \ldots z_{i_r} \star 1 = z_{i_1} \ldots z_{i_r} \\ z_{i_1} \ldots z_{i_r} \star z_{j_1} \ldots z_{j_q} &= z_{i_1}(z_{i_2} \ldots z_{i_r} \star z_{j_1} \ldots z_{j_q}) + z_{j_1}(z_{i_1} \ldots z_{i_r} \star z_{j_2} \ldots z_{j_q}) + z_{i_1+j_1}(z_{i_2} \ldots z_{i_r} \star z_{j_2} \ldots z_{j_q}) \end{aligned}$$

Then, define $\zeta(z_{i_1} \ldots z_{i_r}) := \zeta(i_1, \ldots, i_r)$ and extend ζ by linearity to find:

Proposition 1.4.

$$\zeta(z_{i_1} \ldots z_{i_r})\zeta(z_{j_1} \ldots z_{j_q}) = \zeta(z_{i_1} \ldots z_{i_r} \star z_{j_1} \ldots z_{j_q})$$

Thus we obtain one algebra structure on MZVs. However, it is not the only such structure. We obtain another product on $\mathcal{Z}$ by considering the iterated integral representation of MZVs, an idea going back to Chen [9].

Definition 1.5. Let M be a connected differentiable manifold, and let $\mathcal{P}(M)$ be the set of all paths in M. To be precise, define

$$_x\mathcal{P}(M)_y := \{\gamma : [0,1] \to M | \gamma \text{ piecewise continuous with } \gamma(0) = x,\ \gamma(1) = y\}$$

and

$$\mathcal{P}(M) := \cup_{x,y \in M}\ {_x\mathcal{P}(M)_y}$$

Then, given smooth k-valued 1-forms $\omega_1, \omega_2, \dots, \omega_r$ on M, we define the iterated integral of $\omega_1, \omega_2, \dots, \omega_r$ to be the function

$$\int \omega_1, \omega_2, \dots, \omega_r : \mathcal{P}(M) \to k$$

$$\gamma \mapsto \int_\gamma \omega_1 \omega_2, \dots \omega_r$$

given by

$$\int_\gamma \omega_1, \omega_2, \dots, \omega_r = \int_{0 \le t_1 \le \dots \le t_r \le 1} f_1(t_1) \dots f_r(t_r) dt_1 \dots dt_r$$

where $f_i(t)dt := \gamma^* \omega_i$. We view the constant function 1 as an empty iterated integral.

Remark 1.6. In this thesis, we perform iterated integrals from left to right. It is equally valid, and quite common to work from right to left. Indeed, it is down to the author's personal preference. Similar differences may be found in the definitions of multiple zeta values. Thus, the reader should not worry if another discussion seems at odds with this one

Multiple zeta values may be obtained as iterated integrals on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ as follows

Definition 1.7. Define the 1-form

$$\omega_i := \frac{dz}{z - i}$$

for $i = 0,\ 1$ Then for any binary sequence of the form $w = 10^{s_1-1}10^{s_2-1}1 \dots 10^{s_r-1}$, define the differential form

$$\omega_w = \omega_1 \omega_0^{s_1-1} \dots \omega_1 \omega_0^{s_r-1}$$

Remark 1.8. Similarly to order of integration in iterated integrals, and order of summation in MZVs, the is no standard convention for these ω_i. It is quite common to have this defined as

$$\omega_i := \frac{dz}{i - z}$$

However, the definition given should be consistent with all notions introduced later in this thesis.

Proposition 1.9. *For a binary sequence of the form $w = 10^{s_1-1}10^{s_2-1}1\dots 10^{s_r-1}$, we obtain upon evaluation of the iterated integral of ω_w along the straight line path between 0 and 1*

$$\zeta(s_1,\dots,s_r) = (-1)^r \int \omega_w$$

Remark 1.10. The reader should note that it is common here to introduce the idea of *tangential basepoints*. Roughly speaking, this moves integration to integration over the blowup of our manifold at "problem" points. While this does not particularly alter the analysis, use of tangential basepoints preserves algebraic information that is necessary in the motivic setting. For more detail, we refer the reader to the work of Deligne [11], as a full discussion would fill a thesis.

Example 1.11. Let $w := 100$, then the iterated integral of ω_w is given by

$$\begin{aligned}
\int \omega_1\omega_1\omega_0 &= \int_0^1\int_0^x\int_0^y \frac{dz}{z-1}\frac{dy}{y}\frac{dx}{x} \\
&= -\int_0^1\int_0^x (\int_0^y \sum_{i=0}^{\infty} z^i dz)\frac{dy}{y}\frac{dx}{x} \\
&= -\int_0^1 (\int_0^x \sum_{i=0}^{\infty} \frac{y^i}{i+1} dy)\frac{dx}{x} \\
&= -\int_0^1 \sum_{i=0}^{\infty} \frac{x^i}{(i+1)^2} dx \\
&= -\sum_{i=0}^{\infty} \frac{1}{(i+1)^3} = -\zeta(3)
\end{aligned}$$

Now, by considering the product of two multiple zeta values as iterated integrals, and splitting the domain of integration, we obtain another algebra structure on $\mathcal{Z}$.

Example 1.12.

$$\begin{aligned}
\zeta(2)\zeta(3) &= \int_{0\le z\le y\le x\le 1} \frac{dz}{1-z}\frac{dy}{y}\frac{dx}{x} \int_{0\le t\le s\le 1} \frac{dt}{1-t}\frac{ds}{s} \\
&= \int_{0\le z\le y\le x\le t\le s\le 1} + \int_{0\le z\le y\le t\le x\le s\le 1} + \int_{0\le z\le t\le y\le x\le s\le 1} \\
&+ \int_{0\le t\le z\le y\le x\le s\le 1} + \int_{0\le z\le y\le t\le s\le x\le 1} + \int_{0\le z\le t\le y\le s\le x\le 1} \\
&+ \int_{0\le t\le z\le y\le s\le x\le 1} + \int_{0\le z\le t\le s\le y\le x\le 1} + \int_{0\le t\le z\le s\le y\le x\le 1} \\
&+ \int_{0\le t\le s\le z\le y\le x\le 1} \frac{dz}{1-z}\frac{dy}{y}\frac{dx}{x}\frac{dt}{1-t}\frac{ds}{s} \\
&= 3\zeta(2,3) + \zeta(3,2) + 6\zeta(1,4)
\end{aligned}$$

To make this precise, we consider ζ as a function on $e_1\mathbb{Q}\langle e_0, e_1\rangle e_0$, a sub-vector space of the polynomial algebra in two non-commuting variables as follows:

$$\zeta(e_1 e_0^{s_1-1} e_1 \dots e_1 e_0^{s_r-1}) = \zeta(s_1, \dots, s_r)$$

and extending by linearity. We call monomials in this vector space *convergent words*, and monomials not in this subspace *divergent*.

Definition 1.13. Given two elements of $\mathbb{Q}\langle e_0, e_1\rangle$, define their shuffle product recursively by

$$\begin{aligned} 1 \sqcup\!\sqcup u = u \sqcup\!\sqcup 1 &= u \\ xu \sqcup\!\sqcup yv &= x(u \sqcup\!\sqcup yv) + y(xu \sqcup\!\sqcup v) \end{aligned}$$

where u, v are monomials in e_0, e_1, and $x, y \in \{e_0, e_1\}$.

Proposition 1.14. *For any monomials u, v in $e_1\mathbb{Q}\langle e_0, e_1\rangle e_0$, we have*

$$\zeta(u \sqcup\!\sqcup v) = \zeta(u)\zeta(v)$$

Thus we gain a double algebra structure on $\mathcal{Z}$, in which we additionally obtain the following relation, arising from the involution of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ that interchanges 0 and 1.

Proposition 1.15. *Let $D : \mathbb{Q}\langle e_0, e_1\rangle \to \mathbb{Q}\langle e_0, e_1\rangle$ be the anithomomorphism mapping $e_i \mapsto e_{i+1}$, where indices are considered modulo 2. Then we have $\zeta(w) = \zeta(Dw)$ for all $w \in e_1\mathbb{Q}\langle e_0, e_1\rangle e_0$.*

One might feel that restricting ourselves to the sub-vector space $e_1\mathbb{Q}\langle e_0, e_1\rangle e_0$ is quite limiting, and this is to some extent true. Fortunately, there exist regularisation procedures, one compatible with the shuffle algebra structure and one compatible with the stuffle algebra structure, which allow us to extend ζ to a function on all of $\mathbb{Q}\langle e_0, e_1\rangle$ [22]. Indeed, these regularised MZVs prove critical in providing sufficient relations for conjectured dimensions of the various weight spaces of $\mathcal{Z}$ to hold.

We now mention a few standard conjectures in the theory of MZVs.

Conjecture 1.16. $\mathcal{Z}$ is weight graded: defining $\mathcal{Z}_n := \langle \zeta(s_1, \dots, s_r) | s_1 + \dots + s_r = n\rangle_{\mathbb{Q}}$, we have

$$\mathcal{Z} = \bigoplus_{n=0}^{\infty} \mathcal{Z}_n$$

where we take $\zeta(\varnothing) = 1$.

Conjecture 1.17. The weight graded pieces of $\mathcal{Z}$ have dimensions given by the generating series

$$\sum_{n=0}^{\infty} \dim \mathcal{Z}_n t^n = \frac{1}{1 - t^2 - t^3}$$

Conjecture 1.18. All relations among multiple zeta values can be obtained from the (regularised) shuffle and stuffle relations, alongside the Hoffman relation:

$$\zeta(e_1 \sqcup\!\sqcup u - e_1 \star u) = 0$$

for all convergent u.

1.2 Drinfel'd associators and the KZ equations

In his 1990 work [13] Drinfel'd introduced the idea of an *associator*, a power series in two non-commuting variables.

Definition 1.19. Let k be a field of characteristic 0. A λ-*associator* over a k is an element $\Phi \in k\langle\langle e_0, e_1\rangle\rangle$ that is grouplike for the continuous coproduct

$$\Delta(e_i) = e_i \otimes 1 + 1 \otimes e_i$$

and satisfies the pentagon and hexagon equations

$$\Phi(t_{12}, t_{23} + t_{24})\Phi(t_{13} + t_{23}, t_{34}) = \Phi(t_{23}, t_{34})\Phi(t_{12} + t_{13}, t_{24} + t_{34})\Phi(t_{12}, t_{23})$$

$$\exp(\frac{\pm\lambda e_0}{2})\Phi(e_\infty, e_0)\exp(\pm\frac{\lambda e_\infty}{2})\Phi(e_1, e_\infty)\exp(\pm\frac{\lambda e_1}{2})\Phi(e_0, e_1) = 1$$

where $e_\infty = -e_0 - e_1$ and the t_{ij} are the infinitesimal braid variables, satisfying the following:

$$\begin{aligned} t_{ii} &= 0 \\ t_{ij} &= t_{ji} \\ [t_{ij}, t_{kl}] &= 0 \text{ if i, j, k, l distinct} \\ [t_{ij}, t_{ik} + t_{jk}] &= 0 \text{ if i, j, k distinct} \end{aligned}$$

Together, we refer to these equations as the associator equations.

Interestingly, the hexagon equations are, to some extent, unnecessary, as shown by Furusho [15].

Theorem 1.20 (Furusho)**.** *Let Φ be a grouplike power series in two non commuting variables, satisfying Drinfel'd's pentagon equation. Then there is a unique λ, depending only on the coefficient of the degree 2 terms, such that the pair (λ, Φ) satisfy the hexagon equations.*

While arising originally from the study of quasi-Hopf algebras and braided monoidal categories, associators have since sparked interest in many areas of mathematics, including knot invariants [2], quantum field theory [25], and number theory. In particular, the ties between associators and the Grothendieck-Teichmüller group has drawn much interest.

The Grothendieck-Teichmüller group is quite an important object in algebra, acting on a range of objects in various fields. It exists in three versions: a profinite version, a pro-l version and a pro-unipotent version. The first two are of interest, as the action of the absolute Galois group factors through them, while the latter arises in homological algebra and motivic contexts. It is this last version that appears in the discussion of associators.

Definition 1.21. Define the Grothendieck-Teichmüller group GT to be the affine group scheme over $\mathbb{Q}$, whose k points are given by pairs (λ, f) in $k^\times \times k\langle\langle e_0, e_1\rangle\rangle$ such that

$$\begin{aligned} \Delta f &= f \otimes f \\ f(e_1, e_0) &= f(e_0, e_1)^{-1} \\ f(e_\infty, e_0)e_\infty^{\frac{\lambda-1}{2}} f(e_1, e_\infty)e_1^{\frac{\lambda-1}{2}} f(e_0, e_1)e_0^{\frac{\lambda-1}{2}} &= 1 \\ f(t_{12}, t_{23} + t_{24})f(t_{13} + t_{23}, t_{34}) &= f(t_{23}, t_{34})f(t_{12} + t_{13}, t_{24} + t_{34})f(t_{12}, t_{23}) \end{aligned}$$

where e_∞ and t_{ij} are defined as above. We endow this with a group structure as follows

$$(\lambda, f) \cdot (\lambda', f')(x, y) = (\lambda\lambda', f(x, y)f'(x^\lambda, f^{-1}y^\lambda f))$$

Remark 1.22. The coefficient of e_0e_1 in f nearly determines λ. To be precise, the coefficient is $\frac{\lambda^2}{24}$.

GT acts on the space of associators on the left. We get a similar action on the right by the space of 0-associators,which we call the graded Grothendieck-Teichmüller group GRT, which has product defined by

$$\Phi \cdot \Phi'(e_0, e_1) := \Phi'(e_0, e_1)\Phi(e_0, \Phi'^{-1}e_1\Phi')$$

One can show [13] that the space of associators is a GT-GRT torsor, and hence GT≅GRT. Thus, by studying associators, in particular 0-associators, we can gain information about GT.

One of the first questions one might have about the space of associators is whether it is empty? It is far from obvious that a solution to the associator equations exists for any λ. Drinfeld in fact showed a solution existed and constructed it explicity [13] from the monodromy of the Knizhnik Zamolodchikov equations.

Theorem 1.23 (Drinfel'd)**.** *There exists a solution to the associator equations whose coefficients are given by multiple zeta values*

$$\Phi(e_0, e_1) = \sum_{w \in \langle e_0, e_1\rangle} (-1)^{|w|}\zeta(w)w$$

This adds a further layer of number theoretical interest to the problem of associators, as multiple zeta values are now constrained by the associator equations, giving relations between them. It is in fact conjectured that they describe all non trivial relations between multiple zeta values. However, the associator equations are notoriously challenging, and so the following corollary becomes tremendously useful in describing potential relations among multiple zeta values.

Corollary 1.24. *There exists an associator with coefficients in $\mathbb{Q}$.*

We will not present a proof of this corollary. Should the reader be interested, we recommend either Drinfel'd original work [13], or, if the reader is comfortable with braid theoretic language, Bar-Natan's constructive proof [2].

We will, however, sketch the proof of the theorem, based on the discussion of [29].

Definition 1.25. The Knizhnik Zamolodchikov equations are a system of differential equations

$$\frac{\partial \psi}{\partial x_i} = \sum_{j \neq i} \frac{t_{ij}}{x_i - x_j} \psi$$

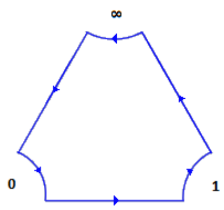
where t_{ij} are defined as above.

Sketch. The connection on $\mathcal{M}_{0,4}$ arising from the KZ equations is given by

$$\nabla = d - t_{12}\frac{dz}{z} - t_{23}\frac{dz}{z-1}$$

Define $\Phi(t_{12}, t_{23})$ to be the holonomy of this connection from $z = 0$ to $z = 1$. We again should consider tangential basepoints here, but we shall gloss over this technicality. Using standard techniques, we compute the holonomy to be

$$\Phi(t_{12}, t_{13}) = \lim_{t \to 0} t^{-t_{23}}(1 + \int_0^1 t_{12}\frac{dt_1}{t_1} + t_{23}\frac{dt_1}{t_1 - 1} + \dots \\ + \int_{0 \leq t_1 \leq \dots \leq t_n \leq 1} (t_{12}\frac{dt_1}{t_1} + t_{23}\frac{dt_1}{t_1 - 1})(\cdots)(t_{12}\frac{dt_n}{t_n} + t_{23}\frac{dt_n}{t_n - 1}) + \dots)t^{t_{12}}$$



To see that this solves the associator equations, we simply consider the holonomy along various paths. For example, the hexagon equations follows from computing the holonomy along the illustrated cycle.

The pentagon equation follows similarly, by integration along a closed curve in $\mathcal{M}_{0,5}$. Then explicitly calculating the integrals gives our result.

We can now discuss the optimistic goals of this project: to find a canonical rational associator. We know that they exist, but none are known explicitly.We even have iterative constructions for rational solutions to the associator equations up to a given weight. However, these constructions involves many choices, and are unlikely to give an explicit formula for the coefficients. Thus begins our problem.

1.3 The double shuffle equations

The first obstruction to finding a rational associator is the difficulty in finding any associator. Thus we will instead attempt to solve a simpler problem: solving the double shuffle equations. We know multiple zeta values satsify a set of shuffle relations, and we expect the associator equations to imply all relations among multiple zeta values. Thus it makes sense to model our easer equations on known MZV relations. In the following definitions, due to Racinet [27], let k be a field. It need not be of characteristic zero, but is normally taken to be.

Definition 1.26. We say a power series $\Phi \in k\langle\langle a, b\rangle\rangle$ solves the shuffle equations if it is grouplike for the completed coproduct for which a, b are primitive. That is

$$\Delta\Phi = \Phi \otimes \Phi$$

where

$$\Delta(x) = x \otimes 1 + 1 \otimes x \text{ for } x = a, b$$

Definition 1.27. Let $Y = y_1, y_2, y_3, \ldots$ be a collection of formal variables. We say a power series $\Phi \in k\langle\langle Y\rangle\rangle$ solves the stuffle equations if it is grouplike for the completed coproduct, defined on generators by

$$\Delta_*(y_n) = \sum_{i=0}^{n} y_i \otimes y_{n-i}$$

where we define $y_0 := 1$.

Definition 1.28. Define the projection map $\pi_Y : k\langle\langle a, b\rangle\rangle \to k\langle\langle Y\rangle\rangle$ to be the linear map given by

$$\pi_Y(ba^{n_1-1}ba^{n_2-1}\ldots ba^{n_k-1}) = y_{n_1}y_{n_2}\ldots y_{n_k}$$

and $\pi_Y(aw) = 0$ for any word $w \in k\langle a, b\rangle$. Define also, for any element $\Phi \in k\langle\langle a, b\rangle\rangle$, $\Phi_{corr} \in k\langle\langle Y\rangle\rangle$ by

$$\Phi_{corr} := \sum_{n\geq 1} \frac{(-1)^n}{n}(\Phi|ba^{n-1})y_1^n$$

where $(\Phi|w)$ denotes the coefficient of w in Φ.

Definition 1.29. We say a power series $\Phi \in k\langle\langle a, b\rangle\rangle$ solves the (regularised) double shuffle equations if Φ solves the shuffle equations and $\Phi^* := \Phi_{corr}\pi_Y(\Phi)$ solves the stuffle equations.

While still challenging to solve, the double shuffle equations are much more tractable, and allow us to make use of additional structures coming from MZVs, such as the depth and weight filtrations. The double shuffle equations are naturally weight graded, for example. Furthermore, it is commonly conjectured that the double shuffle equations describe all possible relations among MZVs, and are hence equivalent to the associator equations. However, little is known about this beyond the work of Furusho [16].

Theorem 1.30. *Let Φ be a grouplike power series in two noncommuting variable. Suppose also that it satisfies the pentagon equation. Then Φ solves the double shuffle equations.*

The space of solutions to the double shuffle equations, denoted DMR, contains a subspace of solutions, DMR_0, such that $(\Phi|e_0) = (\Phi|e_1) = (\Phi|e_0e_1) = 0$. This subspace forms a pro-unipotent group [27] with multiplication given by

$$\Phi \cdot \Phi'(e_0, e_1) := \Phi'(e_0, e_1)\Phi(e_0, \Phi'^{-1}e_1\Phi')$$

which the reader will note is identical to that of GRT. Thus we get the following

Corollary 1.31. *GRT is a subgroup of DMR_0*

It is a standard conjecture that they are in fact equal to the unipotent part of the motivic Galois group, which we shall later discuss in greater depth.

Looking to the shuffle equations has proven quite fruitful, as they also lend themselves well to a rewriting in terms of commutative power series. a technique due to Brown, and very similar to Écalle's theory of moulds [14], this technique has allowed Brown to define a canonical rational associator up to depth 4.

Remark 1.32. From this point in the text, we are interested only in DMR_0, and so we shall assume $(\Phi|e_0) = (\Phi|e_1) = (\Phi|e_0e_1) = 0$ for all potential solutions to the shuffle or stuffle equations.

Definition 1.33. Denote by D_n the vector space spanned by words of depth n in $k\langle a, b\rangle$ and let $\rho_n : D_n \to k[y_0, y_1, \dots, y_n]$ be the isomorphism of vector spaces given by

$$\rho_n(a^{m_0}ba^{m_1}b \dots ba^{m_n}) = y_0^{m_0}y_1^{m_1} \dots y_n^{m_n}$$

The map $\rho := \sum_{n=1}^{\infty} \rho_n$, then defines an isomorphism

$$\begin{aligned} \rho : k\langle a, b\rangle \to \bigoplus_{n=1}^{\infty} k[y_0, \dots y_n] \\ \Phi \mapsto \{\Phi^{(n)}(y_0, \dots, y_n)\}_{n=1}^{\infty} \end{aligned}$$

We can then define the double shuffle equations in this new formulation as polynomial equations.

First we note the following lemma.

Lemma 1.34. *If $\Phi = 1 + \Phi_1 + \Phi_2 + \dots$ solves the shuffle equations, where Φ_n is the depth n component of Φ, then $\rho_n(\Phi_n) \in k[y_0, \dots, y_n]$ is translation invariant.*

Proof. Define $\delta : k\langle a, b\rangle \to k\langle a, b\rangle$ to be the derivation given on generators by

$$\delta(a) := 1$$
$$\delta(b) := 0$$

Note that

$$\delta(a^{m_0}ba^{m_1}b\dots ba^{m_k}) = \sum_{i=0}^{k} m_i a^{m_0}ba^{m_1}b\dots ba^{m_i-1}b\dots ba^{m_k}$$

and that this agrees with the derivation given by $(\pi_0 \otimes id) \circ \Delta$, where $\pi_0(\Phi) := (\Phi|e_0)$. Thus, if $\Delta\Phi = \Phi \otimes \Phi$, we get

$$\delta\Phi = (\Phi|e_0)\Phi = 0$$

But since δ preserves depth, this clearly implies $\delta\Phi_n = 0$. Translating into the language of commutative power series, we get

$$\sum_{i=0}^{n} \frac{\partial}{\partial y_i}\Phi^{(n)} = 0$$

□

In light of this, we lose no information about solutions to the double shuffle equations by setting $y_0 = 0$. Indeed, this is how we shall proceed. In a slight abuse of notation, we shall still refer to the resulting polynomial as $\Phi^{(n)}$. In order to make our discussion unambiguous, we shall adopt the following notational distinction.

$$\Phi^{(n)}(y_0, y_1, \dots, y_n) := \rho_n(\Phi_n)(y_0, \dots, y_n)$$
$$\Phi^{(n)}(x_1, \dots, x_n) := \rho_n(\Phi_n)(0, x_1, \dots, x_n)$$

That is, we will use y_i as variables for the image of ρ, and x_i as variables for the polynomial obtained by setting $y_0 = 0$. We can now define the double shuffle equations in the language of commutative power series.

Definition 1.35. Given a polynomial $f \in k[x_1, \dots, x_n]$, define $f^{\#} \in k[x_1, \dots, x_n]$ by

$$f^{\#}(x_1, \dots, x_n) := f(x_1, x_1 + x_2, x_1 + x_2 + x_3, \dots, x_1 + x_2 + \dots + x_n)$$

We also define recursively the polynomial

$$f(\boldsymbol{x}_1 \dots \boldsymbol{x}_j ⧢ \boldsymbol{x}_{j+1} \dots \boldsymbol{x}_n) :=$$
$$f(\boldsymbol{x}_1(\boldsymbol{x}_2 \dots \boldsymbol{x}_j ⧢ \boldsymbol{x}_{j+1} \dots \boldsymbol{x}_n) + f(\boldsymbol{x}_j(\boldsymbol{x}_1 \dots \boldsymbol{x}_j ⧢ \boldsymbol{x}_{j+2} \dots \boldsymbol{x}_n)$$

where $f(\boldsymbol{x}_1 \dots \boldsymbol{x}_n) := f(x_1, \dots, x_n)$.

Definition 1.36. We say a family of polynomials $\{f^{(n)}\}$ solves the shuffle equations if

$$f^{(n)\#}(\boldsymbol{x}_1 \dots \boldsymbol{x}_j ⧢ \boldsymbol{x}_{j+1}\boldsymbol{x}_n) = f^{(j)}(x_1, \dots, x_j) f^{(n-j)}(x_{j+1}, \dots, x_n)$$

for all $1 \le j < n$.

Defining the stuffle equations is slightly more challenging and requires a few extra definitions

Definition 1.37. For any family of polynomials $\{f^{(n)}\}$, define the operators

$$s_i f^{(r)}(x_1, \dots, x_r) := f^{(r+1)}(x_i, x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_r) \text{ for } 1 \le i \le r$$

Definition 1.38. Define recursively

$$\begin{aligned} f^{(r)}(1 \star \boldsymbol{x}_1 \dots \boldsymbol{x}_r) &= f^{(r)}(\boldsymbol{x}_1 \dots \boldsymbol{x}_r \star 1) = f^{(r)}(x_1, \dots, x_r) \\ f^{(r)}(\boldsymbol{x}_1 \dots \boldsymbol{x}_i \star \boldsymbol{x}_{i+1} \dots \boldsymbol{x}_r) &= s_1 f^{(r-1)}(\boldsymbol{x}_2 \dots \boldsymbol{x}_i \star \boldsymbol{x}_{i+1} \dots \boldsymbol{x}_r) \\ &\quad + s_{i+1} f^{(r-1)}(\boldsymbol{x}_1 \dots \boldsymbol{x}_i \star \boldsymbol{x}_{i+2} \dots \boldsymbol{x}_r) \\ &\quad + \left(\frac{s_1 - s_{i+1}}{x_1 - x_{i+1}} \right) f^{(r-2)}(\boldsymbol{x}_2 \dots \boldsymbol{x}_i \star \boldsymbol{x}_{i+2} \dots \boldsymbol{x}_r) \end{aligned}$$

where $1 \le i \le r$.

Definition 1.39. We say a family of polynomials $\{f^{(n)}\}$ solves the stuffle equations if

$$f^{(n)}(\boldsymbol{x}_1 \dots \boldsymbol{x}_j \star \boldsymbol{x}_{j+1} \boldsymbol{x}_n) = f^{(j)}(x_1, \dots, x_j) f^{(n-j)}(x_{j+1}, \dots, x_n)$$

for all $1 \le j < n$.

Remark 1.40. Note that in this formulation, there is no mention of an analogue to Φ_{corr}. While it is true that we must add a corresponding correction term, we shall ignore this for sake of this discussion. However, we will ask the reader to observe that this arises naturally for multiple zeta values, by considering shuffle regularisation versus stuffle regularisation.

Example 1.41. In depth 2, the double shuffle equations are

$$\begin{aligned} f^{(2)}(x_1, x_1 + x_2) + f^{(2)}(x_2, x_1 + x_2) &= f^{(1)}(x_1) f^{(1)}(x_2) \\ f^{(2)}(x_1, x_2) + f^{(2)}(x_1, x_2) + \frac{f^{(1)}(x_1) - f^{(1)}(x_2)}{x_1 - x_2} &= f^{(1)}(x_1) f^{(1)}(x_2) \end{aligned}$$

while in depth 3, they become

$$\begin{aligned} & f^{(3)}(x_1, x_1 + x_2, x_1 + x_2 + x_3) + f^{(3)}(x_2, x_1 + x_2, x_1 + x_2 + x_3) + f^{(3)}(x_2, x_2 + x_3, x_1 + x_2 + x_3) \\ & \qquad = f^{(1)}(x_1) f^{(2)}(x_2, x_3) \\ & f^{(3)}(x_1, x_2, x_3) + f^{(3)}(x_2, x_1, x_3) + f^{(3)}(x_2, x_3, x_1) + \frac{f^{(2)}(x_1, x_3) - f^{(2)}(x_2, x_3)}{x_1 - x_2} + \frac{f^{(2)}(x_2, x_1) - f^{(2)}(x_2, x_3)}{x_1 - x_3} \\ & \qquad = f^{(1)}(x_1) f^{(2)}(x_2, x_3) \end{aligned}$$

Remark 1.42. From this point onward, we shall often neglect the superscript $f^{(n)}$, instead writing only f, as it should be obvious from the number of variables to which depth we refer.

1.4 The motivic Galois group and the geometry of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$

With such impressive symmetries amongst MZVs, one might hope for some sort of transcendental Galois theory. This is to some extent found in the *motivic* Galois group associated to a certain Tannakian category associated to $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. As general references, the works of Ayoub [1], Deligne [10] and Brown [4],[3] can be useful.

Let $\mathcal{MT}(\mathbb{Z})$ denote the category of mixed Tate motives unramified over $\mathbb{Z}$. THis is a Tannakian category, and hence is equivalent to the category of representations of a group scheme, called its Galois group and denoted by $G_{\mathcal{MT}(\mathbb{Z})}$. $\mathcal{MT}(\mathbb{Z})$ contains as a full Tannakian subcategory $\mathcal{MT}'(\mathbb{Z})$, the Tannakian subcategory generated by the motivic fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. We hence obtain a map

$$G_{\mathcal{MT}(\mathbb{Z})} \to G_{\mathcal{MT}'(\mathbb{Z})}$$

We now define the motivic fundemental group of $X = \mathbb{P}^1 \setminus \{0, 1, \infty\}$, or rather, the motivic fundemental groupoid, of which the motivic fundemental group is a special case.

Definition 1.43. Let x, y be points of $X(\mathbb{C})$. The motivic fundemental groupoid of X consists of the following

- (Betti) A collection of schemes $\pi_1^B(X, x, y)$ defined over $\mathbb{Q}$ and equipped with the structure of a groupoid

  $$\pi_1^B(X, x, y) \times \pi_1^B(X, y, z) \to \pi_1^B(X, x, z)$$

  for any $x, y, z \in X(\mathbb{C})$. There is a natural homomorphism

  $$\pi_1^{top}(X, x, y) \to \pi_1^B(X, x, y)(\mathbb{Q})$$

  where the fundamental groupoid on the left is given by the homotopy classes of paths relative to their endpoints.

- (de Rham) An affine group scheme over $\mathbb{Q}$, denoted by $\pi_1^{dR}(X)$.

- (Comparison) A canonical isomorphism of schemes over $\mathbb{C}$

  $$\text{comp} : \pi_1^B(X, x, y) \times_{\mathbb{Q}} \mathbb{C} \to \pi_1^{dR}(X) \times_{\mathbb{Q}} \mathbb{C}$$

Remark 1.44. We once again gloss over the technicalities of tangential basepoints. For sake of precision, the reader should read $\pi_1^\bullet(X, 0, 1)$ as $\pi_1^\bullet(X, \vec{1}_0, -\vec{1}_1)$ where $\vec{1}_x$ denotes the unit vector parallel to the real line, based at x. Thus, all paths $\gamma : (0, 1) \to \mathbb{C} \setminus \{0, 1\}$ with $\gamma(0) = 0$, $\gamma(1) = 1$ in the following discussion have $\gamma'(0) = -\gamma'(1) = 1$.

Theorem 1.45. *There is an ind-object*

$$\mathcal{O}(\pi_1^{mot}(X, 0, 1)) \in \mathit{Ind}(\mathcal{MT}(\mathbb{Z}))$$

whose Betti and de Rham realisations are the affine rings $\mathcal{O}(\pi_1^B(X, 0, 1))$ *and* $\mathcal{O}(\pi_1^{dR}(X))$ *respectively.*

Define ${}_0\Pi_1 := \mathrm{Spec}(\mathcal{O}(\pi_1^{dR}(X)))$. This is the affine scheme over $\mathbb{Q}$ to which associates to any commutative unitary $\mathbb{Q}$-algebra R the set of grouplike formal power series

$$\{S \in R\langle\langle e_0, e_1\rangle\rangle^\times | \Delta S = S \otimes S\}$$

where Δ is the completed coproduct for which e_i are primitive.

This carries an action of the motivic Galois group $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$, which depends on our choice of basepoints, even though $\pi_1^{dR}(X)$ does not contain an explicit dependence on these points.

Remark 1.46. Among all paths in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ from 0 to 1 satisfying our velocity constraints, there is a distinguished straight line path $\gamma(t) = t$, referred to as the *droit chemin* and denoted *dch*. The natural homomorphism mentioned in Definitions 1.43 maps with onto an element ${}_01_1^B \in \pi_1^B(X, 0, 1)(\mathbb{Q})$. The image of this map under the comparison isomorphism is precisely the Drinfel'd associator

$$\mathrm{comp}({}_01_1^B) = \sum_w \zeta(w)w \in {}_0\Pi_1(\mathbb{C})$$

The action of $G_{\mathcal{MT}(\mathbb{Z})}$ is made more transparent via the decomposition

$$G_{\mathcal{MT}(\mathbb{Z})} = U_{\mathcal{MT}(\mathbb{Z})} \rtimes \mathbb{G}_m$$

into a semidirect product of a pro-unipotent $U_{\mathcal{MT}(\mathbb{Z})}$ and the multiplicative group.

The action of $G_{\mathcal{MT}(\mathbb{Z})}$ restricts to an action

$$U_{\mathcal{MT}(\mathbb{Z})} \times {}_0\Pi_1 \to {}_0\Pi_1$$

which factors through a map

$$\circ^* : {}_0\Pi_1 \times {}_0\Pi_1 \to {}_0\Pi_1$$

called the Ihara action, computed explicitly first by Y. Ihara, but described in [10].

Remark 1.47. We later introduce the *linearised*, or *infinitesimal* Ihara action, in the context of the Lie algebras of DMR_0 and $U_{\mathcal{MT}(\mathbb{Z})}$. The reader must take care to avoid confusing the two.

2 Double Shuffle Modulo Products and Canonical Generators

2.1 The double shuffle Lie algebra

In order to further simplify the equations, we can move from DMR_0 to its Lie algebra $\mathfrak{dmr}_0$, and consider solutions to the double shuffle equations *mod products.*

Definition 2.1. We say $\sigma \in k\langle a, b\rangle$ solves the double shuffle equations mod products if the following hold

$$\begin{aligned} \Delta\sigma &= \sigma \otimes 1 + 1 \otimes \sigma \\ \Delta_*(\sigma^*) &= \sigma^* \otimes 1 + 1 \otimes \sigma^* \\ (\sigma|a) &= (\sigma|b) = (\sigma|ab) = 0 \end{aligned}$$

where $\sigma^* := \pi_Y\sigma + \sigma_{corr}$, where $\sigma_{corr} := \sum_{n\geq 1} \frac{(-1)^n}{n}(\sigma|ba^{n-1})y_1^n$.

Note that the double shuffle equations mod products are homogeneous for weight, and thus we will often assume all monomials in σ to be of the same weight, allowing us to refer to solutions of a particular weight.

Once again, we can rephrase this in terms of commutative variables. We first note the following lemma

Lemma 2.2 (Brown)**.** *If σ solves the shuffle equations, i.e. σ is primitive, then $\rho(\sigma)$ is translation invariant, where ρ is as defined previously.*

Definition 2.3. We say $\{f_j \in k[x_1, \dots, x_j]\}_{j=1}^n$ solves the shuffle equations mod products up to depth $n + 1$ if

$$f_j^{\#}(\boldsymbol{x}_1 \dots \boldsymbol{x}_i ⧢ \boldsymbol{x}_{i+1} \dots \boldsymbol{x}_j) = 0$$

for all $1 \leq i \leq j \leq n$. We say $\{f_j \in k[x_1, \dots, x_j]\}_{j=1}^n$ solves the stuffle equations mod products up to depth $n + 1$ if

$$f_j(\boldsymbol{x}_1 \dots \boldsymbol{x}_i \star \boldsymbol{x}_{i+1} \dots \boldsymbol{x}_j) = 0$$

for all $1 \leq i \leq j \leq n$.

We once again should consider correction terms in the stuffle equations in order to say f solves the double shuffle equations mod products. However, as we may assume f is homogeneous in weight, the correction terms arise only in the depth-equal-to-weight equations, and are easily accounted for. Thus, we say a family of polynomials $\{f_i \in k[x_1, \dots, x_i]\}_{i=1}^n$ is a solution of weight $n+1$ to the double shuffle equations mod products if it solves the shuffle and stuffle equations mod products up to depth $n + 1$.

We now define the Lie algebra structure, which arises via derivations [27] or from the anti-symmetrisation of the Ihara action [5].

Definition 2.4. Given $\psi \in k\langle a, b\rangle$, define the derivation $d_\psi : k\langle a, b\rangle \to k\langle a, b\rangle$ by

$$d_\psi(a) = 0$$
$$d_\psi(b) = [b, \psi]$$

We define the Ihara bracket $\{\cdot, \cdot\} \wedge^2 k\langle a, b\rangle \to k\langle a, b\rangle$ by

$$\{\sigma_1, \sigma_2\} := d_{\sigma_2}\sigma_1 - d_{\sigma_1}\sigma_2 - [\sigma_1, \sigma_2]$$

Alternatively, we can define:

Definition 2.5. Define the linearised Ihara action $\circ : k\langle a, b\rangle \otimes k\langle a, b\rangle \to k\langle a, b\rangle$ by

$$u \circ a^n bv := a^n ubv + a^n bu^* v + a^n b(u \circ v)$$

where, if $u = u_1 u_2 \dots u_r$, $u^* = (-1)^r u_r \dots u_1$ and $u \circ a^n = a^n u$, for all u, v monomials in $k\langle a, b\rangle$, and extend linearly. Define the Ihara bracket by

$$\{\sigma_1, \sigma_2\} = \sigma_1 \circ \sigma_2 - \sigma_2 \circ \sigma_1$$

We then obtain the following from Racinet's thesis.

Proposition 2.6 (Racinet)**.** $\mathfrak{dmr}_0$ *equipped with the Ihara bracket is a Lie algebra. Furthermore, the function*

$$exp_\circ(\sigma) := 1 + \sigma + \frac{1}{2}\sigma \circ \sigma + \frac{1}{6}\sigma \circ \sigma \circ \sigma + \dots$$

defines a map $exp_\circ : \mathfrak{dmr}_0 \to DMR_0$.

The Ihara action, and hence the Ihara bracket are motivic: they arise naturally as from the group structure of $U_{\mathcal{MT}(\mathbb{Z})}$. In fact, one can show $\mathfrak{g} := \mathrm{Lie}(U_{\mathcal{MT}(\mathbb{Z})}) \subset \mathfrak{dmr}_0$ [16], thus the study of $\mathfrak{dmr}_0$ gives us information about both associators and the motivic Galois group. This inclusion is conjecturally an isomorphism of Lie algebras, which gives us a method of generating solutions to the double shuffle equations: we have the non-canonical isomorphism

$$\mathfrak{g} \cong \mathbb{L}(\sigma_3, \sigma_5, \dots)$$

to the free Lie algebra with a generator in every odd degree greater than 1. Thus, given the σ_{2n+1}, we can produce solutions to the double shuffle equations in any weight. However, the σ_{2n+1} are not canonical: we have that

$$\sigma_{2n+1} = \mathrm{ad}(a)(b) + \text{ terms of higher depth}$$

where the adjoint action is with respect to the Lie bracket $[X, Y] = XY - YX$. However, the double shuffle equations give us no power to distinguish between σ_{2n+1} and $\sigma_{2n+1} + \phi$ where $\phi \in \mathfrak{dmr}_0$ is 0 in depth 1. Thus the σ_{2n+1} are ambiguous up to brackets of lower weight elements of $\mathfrak{g}$, limiting their computational use.

2.2 Canonical elements and polar solutions

The first thing one might desire is to make the σ-elements canonical, to have a canonical generating set. There seem to be three main approachs to doing so: using inner products and a Gram-Schmidt-like procedure, using a basis of multiple zeta values, or Brown's anatomical decomposition. The first approach has not been seen in the literature to this point, and so we focus on this, finding several new results.

Theorem 2.7 (Keilthy, Hain)**.** *The generators $\sigma_3, \sigma_5, \sigma_7, \ldots$ of the motivic Lie algebra can be made canonical.*

Proof. Suppose that we have canonical $\sigma_3, \ldots, \sigma_{2k-1}$ and consider the space $\mathbb{L}(\sigma_3, \ldots, \sigma_{2k+1})_{2k+1}$, where the subscript denotes the sub-vector space spanned by elements of weight $2k+1$. This contains $\mathbb{L}(\sigma_3 \ldots, \sigma_{2k-1})_{2k+1}$ as a codimension 1 subspace, and thus, given a non-degenerate inner product, we can fix σ_{2k+1} up to a scalar multiple by imposing orthogonality of σ_{2k+1} to $\mathbb{L}(\sigma_3, \ldots, \sigma_{2k-1})_{2k+1}$. $\square$

There are two natural candidates for our inner product $\langle \cdot, \cdot \rangle : \mathbb{Q}\langle a, b\rangle \times \mathbb{Q}\langle a, b\rangle \to \mathbb{Q}$. Define for monic monomials u, v

$$\langle u, v\rangle_{triv} := \begin{cases} 1 & \text{if } u = v \\ 0, & \text{otherwise} \end{cases}$$

$$\langle u, v\rangle_{\mathcal{S}} := \begin{cases} 1 & \text{if } u = wvw \text{ or } v = wuw \text{ for some } w \in \mathbb{Q}\langle a, b\rangle \\ 0, & \text{otherwise} \end{cases}$$

and extend by linearity. It is easy to check that these satisfy the requirements of inner products.

Example 2.8. By considering the trivial inner product of the depth 3 components of σ_{11} and $\{\sigma_3, \{\sigma_3, \sigma_5\}\}$, and demanding that these be orthogonal, we find the following canonical decomposition of σ_{11}:

$$\begin{aligned}\sigma_{11} = \psi_{11} &- \frac{1}{264}\{\psi_{-1}, \{\psi_{-1}, \psi_{13}\}\} - \frac{241}{2112}\{\psi_9, \{\psi_3, \psi_{-1}\}\} \\ &+ \frac{479}{2112}\{\psi_7, \{\psi_5, \psi_{-1}\}\} - \frac{2053}{6336}\{\psi_5, \{\psi_7, \psi_{-1}\}\} - \frac{2620903}{9649216}\{\sigma_3, \{\sigma_3, \sigma_5\}\} + \ldots\end{aligned}$$

where we have omitted terms of depth 5 (that are uniquely determined), and where ψ_{2n+1} is given by Definition 2.14.

Remark 2.9. One should note that the denominators of coefficients fixed by this method tend to be quite large, with few prime factors. It remains unclear as to whether there is a meaningful reason for this. We suspect it to merely be an artifact of the calculation, as the numbers involves grow quite rapidly.

The first has the advantage of being easy to calculate, with monomials of different weights and depths being orthogonal, while the second is, in some sense,"compatible" with the obvious Lie algebra structure on $\mathbb{Q}\langle a, b\rangle$.

Lemma 2.10 (K.)**.**

$$\langle [w,u], v\rangle_2 + \langle u, [w,v]\rangle_2 = 0 \textit{ for all } u, v, w \in \mathbb{Q}\langle a, b\rangle$$

Proof. Follows simply by considering cases. We shall do an example case, to illustrate the method. We have that the LHS is

$$\langle wu, v\rangle - \langle uw, v\rangle + \langle u, wv\rangle - \langle u, vw\rangle$$

For the first term to be non-zero, we must have $wu = svs$ for some word s. Then either $s = wu'$ or $w = sv'$ where $u = u'u''$ and $v = v'v''$. In the first case, we must have $u'' = vs$. Thus

$$\begin{aligned} u &= u'u'' \\ &= u'vs \\ &= u'vwu' \end{aligned}$$

In the second case, we must then have $u = v''s$. Thus

$$\begin{aligned} vw &= v'v''sv' \\ &= v'uv' \end{aligned}$$

Hence the fourth term is non-zero and cancels out the first. Similarly, if either of the middle brackets are non-zero, so is the other and they cancel each other out. Thus the sum is constantly 0. $\square$

Remark 2.11. While this "symmetric" inner product $\langle\cdot,\cdot\rangle_{\mathcal{S}}$ is compatible with the obvious Lie algebra structure on $\mathbb{Q}\langle a, b\rangle$, it is *not* compatible with the Ihara bracket. Indeed, it would be particularly interesting to find such an inner product. Evidence coming from the work of Pollack [26] suggests the existence of one, but gives no hints as to how to construct it

Remark 2.12. One should note that, while the trivial inner product seems rather unnatural, it actually has Hodge theoretic orgins. It arises from morphism of Lie algebras

$$i : \mathfrak{g} \to \mathrm{Der}^{\Theta}\mathbb{L}(a, b)$$

where Der^{Θ} denotes the set of derivations δ such that $\delta([a, b]) = 0$. This morphism, due to the work of Hain [19] and Brown [7], is known to be injective, and creates further ties to the work of Pollack [26]. To be precise, $i(\sigma_{2n+1}) = \epsilon^{\vee}_{2n+2}$ modulo W_{-2n-3}, where W is the geometric weight filtration associated to the mixed Hodge structure of the first order Tate curve $E^{\times}_{\frac{\partial}{\partial q}}$. Here $\epsilon^{\vee}_{2n} \in \mathrm{Der}^{\Theta}\mathbb{L}(a, b)$ is the derivation defined by

$$\epsilon_{2n}^{\vee}(a) = \mathrm{ad}(a)^{2n}(b) \text{ for } n \geq 1$$

and the fact that it is homogeneous of degree $2n$ in a, b. Defining

$$\epsilon_0^{\vee}(a) = b \; \epsilon_0^{\vee}(b) = 0$$

and denoting by $\mathfrak{u}^{geom}$ the Lie subalgebra generated by the $\epsilon_{2n}^{\vee}$, $n \geq 1$, we obtain the object of study in the work of Pollack. While $i(\mathfrak{g}) \not\subset \mathfrak{u}^{geom}$, in low depth, the epsilons give "coordinates" with which to describe the σ_{2n+1}. Furthermore, the relations between elements of $\mathfrak{u}^{geom}$ give relations between the elements of $\mathfrak{g}$ modulo higher depths, and create ties with the theory of modular forms. This shall be discussed in greater depth later in this thesis.

Another approach to defining canonical generators involves allowing polar solutions to the double shuffle equations [6]:

$$s^{(1)} = \frac{1}{2x_1} \text{ and } s^{(2)} = \frac{1}{12}(\frac{1}{x_1 x_2} + \frac{1}{x_2(x_1 - x_2)})$$

is a solution to the double shuffle equations mod products in depths one and two. By taking the Ihara bracket of s with various solutions, we can define an "anatomical" decomposition for σ_{2k-1}.

Definition 2.13. For any sets of indices $A, B \subset \{0, \ldots, d\}$, write

$$x_{A,B} = \prod_{a \in A, b \in B} (x_a - x_b)$$

If A or B is the empty set, define $x_{A,B} = 1$. Define also $x_0 = 0$

Definition 2.14. For every $n, d \geq 1$, define $\psi_{2n+1}^{(d)} \in \mathbb{Q}(x_1, \ldots x_d)$ by

$$\begin{aligned}\psi_{2n+1}^{(d)} = \frac{1}{2}\sum_{i=1}^{d}(&\frac{(x_i - x_{i-1})^{2n}}{x_{\{0,\ldots,i-2\},\{i-1\}} x_{\{i+1,\ldots,d\},\{i\}}} + \frac{x_d^{2n}}{x_{\{1,\ldots,i-1\},\{0\}} x_{\{i,ldots,d-1\},\{d\}}}) \\ + \frac{1}{2}\sum_{i=1}^{d-1}(&\frac{(x_1 - x_d)^{2n}}{x_{\{2,\ldots,i\},\{1\}} x_{\{i+1,\ldots,d-1,0\},\{d\}}} + \frac{x_{d-1}^{2n}}{x_{\{d,1,\ldots,i-1\},\{0\}} x_{\{i,ldots,d-2\},\{d-1\}}})\end{aligned}$$

Let ψ_{2n+1} be the element whose depth d component is $\psi_{2n+1}^{(d)}$.

Proposition 2.15 (Brown)**.** *ψ_{2n+1} are solutions to the double shuffle equations mod products.*

It is possible to write $\sigma_3, \ldots \sigma_9$ uniquely as Ihara brackets of s and the ψ_{2n+1}. Defining $\psi_{-1} := s$, we can similarly decompose σ_{11}.

Example 2.16.

$$\sigma_{11} = \psi_{11} - \frac{1}{264}\{\psi_{-1},\{\psi_{-1},\psi_{13}\}\} - \frac{241}{2112}\{\psi_9,\{psi_3,\psi_{-1}\}\}$$
$$+ \frac{479}{2112}\{\psi_7,\{\psi_5,\psi_{-1}\}\} - \frac{2053}{6336}\{\psi_5,\{\psi_7,\psi_{-1}\}\} + \{\text{depth } \geq 5\}$$

A priori σ_{11} is only defined up to multiples of $\{\sigma_3,\{\sigma_3,\sigma_5\}\}$. However, by demanding that, in depth three, σ_{11} be written as a sum of brackets $\{\psi_{a_1},\{\psi_{a_2},\psi_{a_3}\}\}$ with at least one of $\{a_1,a_2,a_3\}$ equal to -1, we obtain a canonical generator in weight 11, modulo high depths.

However this approach has only been examined on a case by case basis, with no general theory. Polar solutions still make an appearence in the existence of canonical generators: Brown [7] defines canonical σ_{2k+1} up to depth 3 using polar solutions. To be precise, he defines them as follows.

Definition 2.17. For all $n \geq -1$, define rational functions by

$$\xi^{(1)}_{2n+1} = x_1^{2n}$$
$$\xi^{(2)}_{2n+1} = \{s^{(1)}, x_1^{2n}\}$$
$$\xi^{(3)}_{2n+1} = \{s^{(2)}, x_1^{2n}\} + \frac{1}{2}\{s^{(1)},\{s^{(1)},x_1^{2n}\}\}$$

Note that we can extend ξ_{2n+1} to all depths by $\xi_{2n+1} = \exp(\mathrm{ad}(s))x_1^{2n}$ if we extend s to a solution in all depths.

Definition 2.18. Define canonical generators up to depth three by

$$\sigma^c_{2n+1} = \xi_{2n+1} + \sum_{a+b=n} \binom{2n}{2a} \frac{B_{2a}B_{2b}}{12B_{2n}} \{\xi_{2a+1},\{\xi_{2b+1},\xi_{-1}\}\}$$

where B_{2n} is the $2n^{th}$ Bernoulli number.

In [7], Brown shows the following

Proposition 2.19 (Brown)**.** *σ^c_{2n+1} solve the double shuffle equations mod products up to depth three, and have no poles, thus defining genuine elements of $\mathfrak{dmr}_0$.*

These generators give interesting ties to $\mathfrak{sl}_2$ and period polynomials, that also arise in the work of Pollack [26]. Specifically, the coefficients appearing in the expression are proportional to those of the odd part of the period polynomial for the Eisenstein series of weight $2n$, which is proportional to:

$$\sum_{a+b=n,\ a,b\geq 1} \binom{2n}{2a} B_{2a}B_{2b}X^{2a-1}Y^{2b-1} \ \in\ \mathbb{Q}[X,Y]$$

One thing of note would be if an inner product produced the same canonical generators as one of the other methods. We have checked that the "anatomical" decomposition, and the trivial inner product give distinct generators, but it has yet to be checked in other cases.

2.3 The duality phenomenon

One phenomenon amongst elements of $\mathfrak{dmr}_0$ is that of *duality.*

Definition 2.20. Define the following linear maps on $\mathbb{Q}\langle a, b\rangle$

- $R(u_1 u_2 \dots u_n) := u_n u_{n-1} \dots u_1$
- S is the homomorphism defined by $Sa := b$ and $Sb := a$
- $\mathrm{D} := RS = SR$

We say σ satisfies *duality* if $\sigma = \mathrm{D}\sigma$

We have $\zeta(w) = \zeta(\mathrm{D}w)$, which we expect: this is just swapping the roles of 0 and 1 in $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. What is unexpected is that we seem to have $\sigma = \mathrm{D}\sigma$ for all $\sigma \in \mathfrak{dmr}_0$. It is not currently known if duality is a consequence of the double shuffle relations, but numerical evidence seems to suggest it must be.

Remark 2.21. The map S defined here is, up to a sign, the antipode map in the shuffle Hopf algebra $\mathbb{Q}\langle a, b\rangle$.

We do, however, know that duality plays nicely with many of the structures on $\mathfrak{dmr}_0$: D passes through the motivic coaction [4] and duality is preserved by the Ihara bracket. While this latter fact follows from Brown's proof that the Ihara action is motivic [5], and Racinet's thesis [27], we present a direct proof of it.

Lemma 2.22 (K.). *If $\phi(a, b) \in \mathbb{Q}\langle a, b\rangle$ satisfies the shuffle equations mod products, then $D\phi(a, b) = -\phi(-b, -a)$*

Proof. If $\phi(a, b)$ satisfies the shuffle equations mod products, we must have

$$\phi(a, b) + R\phi(-a, -b) = 0$$

Applying D to this proves our result. $\square$

Theorem 2.23 (K.). *Duality is preserved in $\mathfrak{dmr}_0$ by the Ihara bracket*

Proof. The Ihara bracket of two elements is defined by

$$\{\phi_1, \phi_2\} := d_{\phi_2}\phi_1 - d_{\phi_1}\phi_2 - [\phi_1, \phi_2]$$

where d_ϕ is the derivation defined on generators by

$$d_\phi(a) = 0$$

$$d_\phi(b) = [b, \phi]$$

Now suppose $\phi_1, \phi_2 \in \mathfrak{dmr}_0$ satisfy duality, and consider $\{\phi_1, \phi_2\}(-b, -a)$ We have the following:

$$[\phi_1, \phi_2](-b, -a) = [\phi_1, \phi_2]$$

Next define a derivation d'_ϕ by

$$d'_\phi(a) = [a, \phi]$$

$$d_\phi(b)' = 0$$

We can easily show by induction on the length of ϕ that $d_\phi(X)(-b,-a) = d'_\phi(X(-b,-a))$ and hence

$$d_{\phi_i}(\phi_j)(-b,-a) = -d'_{\phi_i}(\phi_j) \text{ for } (i,j) \in \{(1,2);(2,1)\}$$

One can then check easily that $d'_\phi(X) = d_\phi(X) - [X, \phi]$, by induction, and hence

$$(d_{\phi_1}(\phi_1) - d_{\phi_2}(\phi_1))(-b,-a) = -d_{\phi_1}(\phi_1) + d_{\phi_2}(\phi_1) + 2[\phi_1, \phi_2]$$

and so $\mathrm{D}\{\phi_1, \phi_2\} = -\{\phi_1, \phi_2\}(-b,-a) = \{\phi_1, \phi_2\}$ □

We can also make steps towards a proof that duality holds for all elements of $\mathfrak{dmr}_0$. To be precise, we can show that it holds for elements of $\mathfrak{g}$, with minor assumptions. It in fact follows from the definition. However, we once again provide a more direct proof, as the proof, with some further assumptions, extend to $\mathfrak{dmr}_0$. We first note that D preserves solutions to the shuffle equations.

Lemma 2.24 (K.). *If $\phi(a,b) \in \mathbb{Q}\langle a,b\rangle$ satisfies the shuffle equations mod products, then so does $D\phi$.*

Proof. One can easily check that

$$(R \otimes R) \circ \Delta = \Delta \circ R$$

and

$$(S \otimes S) \circ \Delta = \Delta \circ S$$

Thus

$$(\mathrm{D} \otimes \mathrm{D}) \circ \Delta = \Delta \circ \mathrm{D}$$

proving our result. □

We can now show the following.

Proposition 2.25 (K.). *Suppose $\sigma_3, \ldots, \sigma_{2k-1}$ satisfy duality. Suppose also that $\mathrm{D}\sigma_{2k+1} \in \mathfrak{g}$. Then σ_{2k+1} satisfies duality.*

Proof. By our assumption, $\mathrm{D}\sigma_{2k+1}$ must be in the span of σ_{2k+1} and brackets of lower weight generators. Thus, there exists $\alpha \in \mathbb{Q}$ such that $\sigma_{2k+1} - \alpha\mathrm{D}\sigma_{2k+1}$ is a linear combination of brackets of lower weight generators. By the previous theorem, $\sigma_{2k+1} - \alpha\mathrm{D}\sigma_{2k+1}$ must satisfy duality and thus

$$(\alpha + 1)\sigma_{2k+1} = (\alpha + 1)\mathrm{D}\sigma_{2k+1}$$

Then, as $\mathfrak{g} \subset \mathfrak{dmr}_0$, we obtain from the stuffle equation and translation invariance of σ_{2k+1}, evaluated at $x_1 = 1$, $x_i = 0$ $i = 2, 3, ..., 2k$, that

$$\begin{aligned}(\sigma_{2k+1}|ab^{2k}) &= -(\sigma_{2k+1}|bab^{2k-1}) - (\sigma_{2k+1}|b^2ab^{2k-2}) - \cdots - (\sigma_{2k+1}|b^{2k}a) \\ &= \sum_{i=1}^{2k-1}(\sigma_{2k+1}|b^ia^2b^{2k-1-i}) \\ &\vdots \\ &= (-1)^{2k}(\sigma_{2k+1}|b^{2k}a) = (\sigma_{2k+1}|a^{2k}b)\end{aligned}$$

and so

$$(\mathrm{D}\sigma_{2k+1}|a^{2k}b) = (\sigma_{2k+1}|ab^{2k}) = (\sigma_{2k+1}|a^{2k}b)$$

Thus, we must have $\alpha = 1$ and so $\sigma_{2k+1} = \mathrm{D}\sigma_{2k+1}$ □

One could alter the assumptions made about $\mathrm{D}\sigma_{2k+1}$, however, it is not clear that the altered assumptions would be weaker. For example, if we simply take $\mathrm{D}\sigma_{2k+1} \in \mathfrak{dmr}_0$ [30] we have to make certain assumptions about the nature of $\mathfrak{dmr}_0$ in order to follow the same proof method. Note also that we cannot replace σ_{2k+1} by an arbirtrary element, as we rely on having non-zero depth one components, and in this, σ-elements are near unique in $\mathfrak{dmr}_0$.

We also get an interesting interplay between duality and the proposed symmetric inner product.We first note the following trivial fact.

Lemma 2.26 (K.)**.**

$$\langle Du, Dv\rangle_{\mathcal{S}} = \langle u, v\rangle_{\mathcal{S}}$$

Definition 2.27. Given an inner product $\langle\cdot,\cdot\rangle_{\mathcal{S}}$, define

$$\langle u, v\rangle_m = \begin{cases} \langle u, v\rangle_{\mathcal{S}} & \text{if } u, v \text{ are both of odd depth} \\ -\langle u, v\rangle_{\mathcal{S}} & \text{if } u, v \text{ are both of even depth} \\ 0 & \text{otherwise} \end{cases}$$

Definition 2.28. Define $\mathbb{Q}^o\langle a, b\rangle$ to be the subspace of $\mathbb{Q}\langle a, b\rangle$ consisting of polynomials with monomials only of odd weight.
Let $\mathbb{Q}^D\langle a, b\rangle$ be the subspace of $\mathbb{Q}^o\langle a, b\rangle$ consisting of polynomials equal to their duals.
Let $\mathbb{Q}^O\langle a, b\rangle$ be the subspace of $\mathbb{Q}^o\langle a, b\rangle$ consisting of polynomials with monomials only of odd depth. Note that we have a surjection $\pi : \mathbb{Q}^D\langle a, b\rangle \to \mathbb{Q}^O\langle a, b\rangle$.

Lemma 2.29 (K.)**.** *$\langle\sigma, \rho\rangle_m = 0$ for all $\sigma, \rho \in \mathbb{Q}^D\langle a, b\rangle$.*

Proof. We have

$$\langle\sigma, \rho\rangle_m = \langle\sigma_{odd}, \rho_{odd}\rangle_{\mathcal{S}} - \langle\sigma_{even}, \rho_{even}\rangle_{\mathcal{S}}$$

As duality swaps the parity of depth of elements of $\mathbb{Q}^o\langle a, b\rangle$, we get that

$$\begin{aligned}\langle\sigma, \rho\rangle_m &= \langle\sigma_{odd}, \rho_{odd}\rangle_{\mathcal{S}} - \langle D\sigma_{odd}, D\rho_{odd}\rangle_{\mathcal{S}} \\ &= \langle\sigma_{odd}, \rho_{odd}\rangle_{\mathcal{S}} - \langle\sigma_{odd}, \rho_{odd}\rangle_{\mathcal{S}} = 0\end{aligned}$$

□

Lemma 2.30 (K.)**.** *If* $\langle \sigma, \rho \rangle_m = 0$ *for all* $\rho \in \mathbb{Q}^D\langle a, b\rangle$*, then* $\sigma \in \mathbb{Q}^D\langle a, b\rangle$*.*

Proof.

$$\begin{aligned} \langle \sigma, \rho \rangle_m = 0 \ \forall \ \rho \in \mathbb{Q}^D\langle a, b\rangle &\Rightarrow \langle \sigma_{odd}, \rho_{odd} \rangle_{\mathcal{S}} = \langle \sigma_{even}, \rho_{even} \rangle_{\mathcal{S}} \ \forall \ \rho \in \mathbb{Q}^D\langle a, b\rangle \\ &\Rightarrow \langle \sigma_{odd}, \rho_{odd} \rangle_{\mathcal{S}} = \langle D\sigma_{even}, \rho_{odd} \rangle_{\mathcal{S}} \ \forall \ \rho \in \mathbb{Q}^D\langle a, b\rangle \\ &\Rightarrow \langle \sigma_{odd} - D\sigma_{odd}, \rho_{odd} \rangle_{\mathcal{S}} = 0 \ \forall \ \rho_{odd} \in \mathbb{Q}^O\langle a, b\rangle \end{aligned}$$

Then, as $\langle \cdot, \cdot \rangle_{\mathcal{S}}$ is a nondegenerate inner product on $\mathbb{Q}^O\langle a, b\rangle$, we must have

$$\sigma_{odd} = D\sigma_{even}$$

which implies

$$\sigma = D\sigma$$

as $D^2 = D$. □

Theorem 2.31 (K.)**.**

$$\mathbb{Q}^D\langle a, b\rangle = \cap_{\rho \in \mathbb{Q}^D\langle a,b\rangle} ker\langle \cdot, \rho \rangle_{\mathcal{S}}$$

So the symmetric inner product in some sense "cuts out" polynomials satisfying duality. Unfortunately, this fact is computationally ineffective, but still interesting.

2.4 Linearised double shuffle equations

While the double shuffle equations are homogeneous for weight, they are not homogeneous for depth. Rather, the shuffle equations are, but the stuffle equations are not. As such, we can further simplify our equations by taking the associated graded of $\mathfrak{dmr}_0$ with respect to the depth filtration, to obtain $\mathfrak{dg}$. This is no longer a free Lie algebra, as we now obtain relations among $\bar{\sigma}_{2i+1}$, the images of σ_{2n+1}, identical to those of Pollack [26]. However, the equations describing elements of $\mathfrak{dg}$ become much simpler. Indeed, we have $\mathfrak{dg} \subset \mathfrak{ls}$, the space of solutions to the *linearised double shuffle equations* [5].

Definition 2.32. We say $\sigma \in k\langle a, b\rangle$ satisfies the linearised double shuffle equations if the following conditions hold:

$$\begin{aligned} \Delta\sigma &= \sigma \otimes 1 + 1 \otimes \sigma \\ \Delta_*^{\mathfrak{ls}} \pi_Y \sigma &= \pi_y \sigma \otimes 1 + 1 \otimes \pi_Y \sigma \\ (\sigma|a) &= (\sigma|b) = (\sigma|ab) = 0 \end{aligned}$$

where $\Delta_*^{\mathfrak{ls}} : k\langle Y\rangle \to k\langle Y\rangle \otimes k\langle Y\rangle$ is defined on generators by

$$\Delta_*^{\mathfrak{ls}}(y_i) := y_i \otimes 1 + 1 \otimes y_i$$

We denote the space of solutions to the linearised double shuffle equations by $\mathfrak{ls}$.

Proposition 2.33 (Brown)**.** $\mathfrak{ls}$ *equipped with the Ihara bracket forms a Lie algebra.*

We can once again translate this into the language of commutative variables.

Definition 2.34. We say $f \in k[x_1, \ldots, x_n]$ solves the linearised double shuffle equations if

$$
\begin{aligned}
f^{\#}(\boldsymbol{x}_1 \ldots \boldsymbol{x}_i \sqcup\!\sqcup \boldsymbol{x}_{i+1} \ldots \boldsymbol{x}_n) &= 0 \\
f(\boldsymbol{x}_1 \ldots \boldsymbol{x}_i \sqcup\!\sqcup \boldsymbol{x}_{i+1} \ldots \boldsymbol{x}_n) &= 0
\end{aligned}
$$

Remark 2.35. Note that we have $\sqcup\!\sqcup$ in both the linearised shuffle and linearised stuffle equations. The primary distinction between $\sqcup\!\sqcup$ and $\star$ is the lower depth terms, which disappear in the linearisation.

Remark 2.36. Note that we can now assume $\sigma \in \mathfrak{ls}$ to be homogeneous in weight *and* depth, as our equations are now homogeneous in both.

While it is not immediately obvious that moving to the linearised double shuffle equations achieves anything of note, one can translate several important conjectures into conjectures about the nature of $\mathfrak{dg}$ and $\mathfrak{ls}$. For example, Brown [5] defines an explicit injective linear map

$$\mathbf{e} : \mathrm{S}_{2n} \to \mathfrak{ls}$$

where $\mathrm{S}_{2n} \subset \mathbb{Q}[X, Y]$ is the vector space of even period polynomials.

Definition 2.37. Define $\mathrm{S}_{2n} \subset \mathbb{Q}[X, Y]$ to be the vector space of antisymmetric homogeneous polynomials $P(X, Y)$ of degree $2n - 2$ satisfying

$$
\begin{gathered}
P(X, 0) = 0 \\
P(\pm X, \pm Y) = P(X, Y) \\
P(X, Y) + P(X - Y, X) + P(-Y, X - Y) = 0
\end{gathered}
$$

This map provides a reformulation of the (depth graded) Broadhurst-Kreimer conjecture on the dimensions of $\mathfrak{dg}$:

Conjecture 2.38. The image of $\mathbf{e}$ lies in $\mathfrak{dg}$ and

$$
\begin{aligned}
H_1(\mathfrak{dg}; \mathbb{Q}) &\cong \bigoplus_{i \geq 1} \bar{\sigma}_{2i+1}\mathbb{Q} \oplus \bigoplus_{n \geq 1} (e)(\mathrm{S}_{2n}) \\
H_2(\mathfrak{dg}; \mathbb{Q}) &\cong \bigoplus_{n \geq 1} \mathrm{S}_{2n} \\
H_i(\mathfrak{dg}; \mathbb{Q}) &= 0 \text{ for all } i \geq 3
\end{aligned}
$$

This can be made into a much stronger conjecture about the homology of $\mathfrak{ls}$.

Conjecture 2.39. Denoting by $\mathfrak{ls}_1$ the depth 1 component of $\mathfrak{ls}$, and by $\mathrm{S} := \bigoplus_{n \geq 1} \mathrm{S}_{2n}$, it is conjectured that the following holds:

$$
\begin{aligned}
H_1(\mathfrak{ls}; \mathbb{Q}) &\cong \mathfrak{ls}_1 \oplus \mathbf{e}(\mathrm{S}) \\
H_2(\mathfrak{ls}; \mathbb{Q}) &\cong \mathrm{S} \\
H_i(\mathfrak{ls}; \mathbb{Q}) &= 0 \text{ for all } i \geq 3
\end{aligned}
$$

Conjecturally, these are equivalent: it is believed that $\mathfrak{dg} \cong \mathfrak{ls}$. Both would imply the following conjecture on the dimensions of $\mathfrak{dg}$.

Conjecture 2.40. Denoting by $\mathcal{D}$ the depth filtration, we have

$$\sum_{N,d>0} \dim_{\mathbb{Q}}(\mathrm{gr}_d^{\mathcal{D}} \mathcal{Z}_N) s^N t^d = \frac{1+\mathbb{E}(s)t}{1-\mathbb{O}(s)t+\mathbb{S}(s)t^2-\mathbb{S}(s)t^4}$$

where

$$\mathbb{E}(s) = \frac{s^2}{1-s^2} \ , \ \mathbb{O}(s)\frac{s^3}{1-s^2} \ , \ \mathbb{S}(s)\frac{s^12}{(1-s^4)(1-s^6)}$$

Here $\mathbb{E}(s)$ and $\mathbb{O}(s)$ are the generating series of the dimensions of spaces of even and odd single zeta values respectively. $\mathbb{S}(s)$ has an interpretation as the generating series for the graded dimensions of the space of cusp forms for the full modular group $PSL_2(\mathbb{Z})$.

This conjecture makes the connection with period polynomials and modular forms slightly more explicit. However, it is not clear precisely why the connection exists.

Still, the study of solutions to the linearised double shuffle equations gives powerful machinery, such as the depth-parity theorem [5].

Proposition 2.41. *Suppose $\sigma \in \mathfrak{ls}$ is of weight N and depth d. Then, if N and d are of opposite parity, $\sigma = 0$. That is, there are no non-trivial solutions to the linearised double shuffle equations with weight and depth of opposite parity.*

This in turn gives use a method for tackling so called "totally odd" multiple zeta values [5],[12]. Multiple lower bounds for the dimensions of the space of totally odd multiple zeta values have been given. However, as the notation involved is quite particular, we mention this only as an aside.

Another useful corollary of the depth parity theorem is the following.

Corollary 2.42. *For a solution to the double shuffle equations mod products $\phi \in \mathfrak{dmr}_0$, of weight N, the depth $d+1 \not\equiv N$ (mod 2) components are uniquely determined by the lower depths. In particular, σ_{2n+1} is uniquely determined in depths 1 and 2.*

Proof. Suppose ϕ_1 and ϕ_2 are of weight N and agree up to depth $d \equiv N$ (mod 2). Then the depth $d+1$ component of $\phi_1 - \phi_2$ is a solution to the linearised double shuffle equations and hence, by the depth parity theorem, is 0. Thus ϕ_1 and ϕ_2 agree up to depth $d+1$ and the depth $d+1$ compenent is uniquely determined. $\square$

Remark 2.43. It would be interesting if this corollary could be "dualised": if we assume that the duality operator preserves $\mathfrak{dmr}_0$, then we must have that the depth $d-1 \not\equiv N$ (mod 2) component of a weight N element of $\mathfrak{dmr}_0$ is uniquely determined by the higher depths, suggesting that a top down approach may be a viable option in solving the double shuffle equations mod products.

3 Motivic Multiple Zeta Values and Additional Structures

3.1 Goncherov and Brown's motivic iterated integrals

Similar our earlier notation for iterated integrals, we introduce the following definition.

Definition 3.1. Define $I(a_0; a_1, a_2, \dots, a_n; a_{n+1}$ to be the iterated integral of $\omega_{a_1} \dots \omega_{a_n}$ along the straight line path from a_0 to a_{n+1}, where we define

$$\omega_a := \frac{dz}{z-a}$$

Also define the *weight* of such an iterated integral to be n.

Remark 3.2. Note that, taking $a_0 = 0$, $a_{n+1} = 1$, we recover our definition of multiple zeta values by iterated integrals. Once again, we gloss over the technicalities of tangential basepoints.

These satisfy the following, easily verified properties.

- $I(a_0; a_1, \dots, a_n; a_0) = 0$
- (Reversal of Paths)$I(a_0; a_1, \dots, a_n; a_{n+1}) = (-1)^n I(a_{n+1}; a_n, \dots, a_1; a_0)$
- (Functoriality)$I(a_0; a_1, \dots, a_n; a_{n+1}) = I(1-a_0; 1-a_1, \dots, 1-a_n; 1-a_{n+1})$
- (Shuffle regularisation)

$$(-1)^k I(0; \{0\}^k, 1, \{0\}^{n_1-1}, \dots, 1, \{0\}^{n_r-1}; 1) = \sum_{i_1+\dots+i_r=k} \binom{n_1-1+i_1}{i_1} \dots \binom{n_r-1+i_r}{i_r} I(0; 1, \{0\}^{n_1+i_1-1}, \dots, 1, \{0\}^{n_r+i_r-1}; 1)$$

Goncharov [18] defines a motivic analogue of these iterated integrals, denoted $I^{\mathfrak{a}}(a_0; a_1, \dots, a_n; a_{n+1})$, as elements of a $\mathbb{Q}$-algebra, satisfing the above mentioned properties of iterated integrals and with the following coproduct.

Definition 3.3. Let $\mathcal{I}$ denote the $\mathbb{Q}$-algebra generated by Goncharov's motivic iterated integrals, and define the map

$$\Delta : \mathcal{I} \to \mathcal{I} \otimes \mathcal{I}$$

by

$$\Delta I^{\mathfrak{a}}(a_0; a_1, \dots, a_n; a_{n+1}) := \sum_{0=i_0<i_1<\dots<i_k<i_{k+1}=n+1} \prod_{p=0}^{k} I^{\mathfrak{a}}(a_{i_p}; a_{i_p+1}, \dots, a_{i_{p+1}-1}; a_{i_{p+1}}) \otimes I^{\mathfrak{a}}(a_0; a_{i_1}, \dots, a_{i_k}; a_{n+1})$$

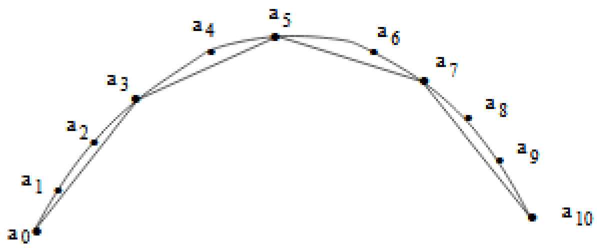
where $0 \leq k \leq n$.

The terms in the above formula are in one-to-one correspondence with the subsequences

$$\{a_{i_1}, \dots, a_{i_k}\} \subset \{a_1, \dots, a_n\}$$

To be more precise, every term corresponds to a polygon with verticles at the points a_i inscribed into a semicircle.

Example 3.4. The polygon



corresponds to the term

$$I^{\mathfrak{a}}(a_0; a_1, a_2; a_3) I^{\mathfrak{a}}(a_3; a_4; a_5) I^{\mathfrak{a}}(a_5; a_6; a_7) I^{\mathfrak{a}}(a_7; a_8, a_9; a_{10}) \otimes I^{\mathfrak{a}}(a_0; a_3, a_5, a_7; a_{10})$$

The additional algebraic structure arising from this coproduct proves to be an incredibly powerful tool, as we shall soon see.

By restricting the a_i to $\{0, 1\}$, we obtain Goncharov's *motivic multiple zeta values*, $\zeta^{\mathfrak{a}}(n_1, \dots, n_k)$, with the two notations related as for standard MZVs. Noting that $I^{\mathfrak{a}}(0; 1, 0; 1) = \zeta^{\mathfrak{a}}(2) = 0$, we obtain a "period map", from the space of Goncharov motivic MZVs $\mathcal{A}$ to $\mathcal{Z}/\zeta(2)$:

$$\begin{aligned} \mathrm{per}^{\mathfrak{a}} : \mathcal{A} &\to \mathcal{Z}/\zeta(2) \\ \zeta^{\mathfrak{a}}(n_1, \dots, n_k) &\mapsto \zeta(n_1, \dots, n_k) + \zeta(2)\mathcal{Z} \end{aligned}$$

Brown [4] similarly defines a motivic iterated integral $I^{\mathfrak{m}}(a_0; a_1, \dots, a_n; a_{n+1})$, which we shall not discuss in any great detail, that extends Goncharov's definition to one in which $\zeta^{\mathfrak{m}}(2)$ is non zero. They still satisfy all aforementioned properties and, denoting the space of Brown's motivic multiple zeta values by $\mathcal{H}$, we obtain an extension of Goncharov's period map:

$$\begin{aligned} \mathrm{per} : \mathcal{H} &\to \mathcal{Z} \\ \zeta^{\mathfrak{m}}(n_1, \dots, n_k) &\mapsto \zeta(n_1, \dots, n_k) \end{aligned}$$

Furthermore, we can also lift Goncharov's coproduct to a coaction on the space $\mathcal{H}$ of Brown's motivic iterated integrals

$$\Delta : \mathcal{H} \to \mathcal{A} \otimes \mathcal{H}$$

using precisely Goncharov's formula. This coaction filters through certain infinitesimal coactions.

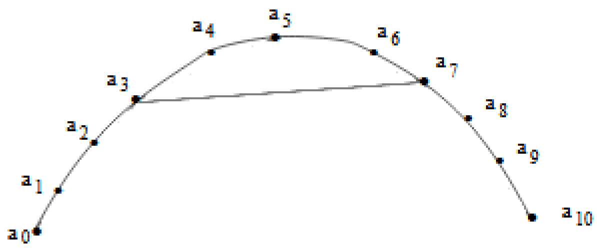
Definition 3.5. Let $\mathcal{H}_N$ be the subspace of $\mathcal{H}$ consisting of elements of weight N, and let $\mathcal{L}_r$ be the weight r component of $\mathcal{L} := \mathcal{A}_{>0}/\mathcal{A}_{>0}\mathcal{A}_{>0}$. We then define, for $1 \leq r < N$

$$D_r : \mathcal{H}_N \to \mathcal{L}_r \otimes \mathcal{H}_{N-r}$$
$$I^{\mathfrak{m}}(a_0; a_1, \ldots, a_N; a_{N+1}) \mapsto \sum_{p=0}^{N-r} I^{\mathfrak{a}}(a_p; a_{p+1}, \ldots, a_{p+r}; a_{p+r+1}) \otimes I^{\mathfrak{m}}(a_0; a_1, \ldots, a_p, a_{p+r+1}, \ldots, a_N; a_{N+1})$$

where $I^{\mathfrak{a}}$ is taken to be its projection into $\mathcal{L}$.

This can similarly be represented by considering segments between points on a semi-circle.

Example 3.6. The picture



corresponds to the term

$$I^{\mathfrak{a}}(a_3; a_4, a_5, a_6; a_7) \otimes I^{\mathfrak{a}}(a_0; a_1, a_2, a_3, a_7, a_8, a_9; a_{10})$$

in $D_3(I^{\mathfrak{a}}(a_0; a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8, a_9; a_{10}))$.

We then have the following theorem, due to Brown [4].

Theorem 3.7 (Brown)**.** *The kernel of $D_{<N} := \oplus_{3 \leq 2r+1 < N} D_{2r+1}$ is $\zeta^{\mathfrak{m}}(N)\mathbb{Q}$ in weight N.*

Example 3.8. We will compute D_3 of $4\zeta^{\mathfrak{m}}(2,3) + 6\zeta^{\mathfrak{m}}(3,2)$.

$$\begin{aligned}
D_3(\zeta^{\mathfrak{m}}(2,3) &= D_3(I^{\mathfrak{m}}(0;1,0,1,0,0;1)) \\
&= I^{\mathfrak{a}}(1;0,1,0;0) \otimes I^{\mathfrak{m}}(0;1,0;1) + I^{\mathfrak{a}}(0;1,0,0;1) \otimes I^{\mathfrak{m}}(0;1,0;1) \\
D_3(\zeta^{\mathfrak{m}}(3,2) &= D_3(I^{\mathfrak{m}}(0;1,0,0,1,0;1)) \\
&= I^{\mathfrak{a}}(0;1,0,0;1) \otimes I^{\mathfrak{m}}(0;1,0;1) + I^{\mathfrak{a}}(1;0,0,1;0) \otimes I^{\mathfrak{m}}(0;1,0;1) \\
&+ I^{\mathfrak{a}}(0;0,1,0;1) \otimes I^{\mathfrak{m}}(0;1,0;1) \\
D_3(\zeta^{\mathfrak{m}}(2)\zeta^{\mathfrak{m}}(3) &- \zeta^{\mathfrak{m}}(2,3) - \zeta^{\mathfrak{m}}(3,2)) = 0
\end{aligned} \tag{1}$$

using shuffle renormalisation and reversal of paths. Thus, we must have that $4\zeta^{\mathfrak{m}}(2,3) + 6\zeta^{\mathfrak{m}}(3,2) = \alpha\zeta^{\mathfrak{m}}(5)$ for some $\alpha \in \mathbb{Q}$.

Using this machinery, Brown goes on to show the following theorem.

Theorem 3.9 (Brown)**.** *In weight N, $\mathcal{H}_N$ has basis $\zeta^{\mathfrak{m}}(a_1, \dots, a_n)$ where $a_i \in \{2, 3\}$.*

This basis is called the *Hoffman basis*, and the corresponding zeta values are called Hoffman zeta values. Partially confirming a conjecture due to Hoffman, this theorem has the following immediate corollaries.

Corollary 3.10. *In weight N, $\mathcal{Z}_N$ is spanned by $\zeta(a_1, \dots, a_n)$, where $a_i \in \{2, 3\}$.*

Corollary 3.11.

$$\sum_{N=0}^{\infty} dim\ \mathcal{H}_N t^N = \frac{1}{1 - t^2 - t^3}$$

As motivic multiple zeta values, and the motivic coproduct are such powerful tools, demanding that any algebraic structure we impose on MZVs be compatible with the motivic theory is not an unreasonable starting point. For example, the weight filtration is motivic, and from earlier discussion, we can see that it is a grading for motivic MZVs, and weight is preserved in all known relations. The depth filtration is motivic, but not a grading. However, it seems that depth graded motivic multiple zeta values may not be the most natural objects to study. A more natural option is a filtration arising from a decomposition due to Charlton [8]: the block filtration.

3.2 The block decomposition of MZVs

Call a word in e_0, e_1 *alternating* if it is non-empty and has no subsequences of the form e_0e_0 or e_1e_1. There are exactly two alternating words of a given length:

$$A = \{e_0, e_1, e_0e_1, e_1e_0, e_0e_1e_0, e_1e_0e_1, \dots\}$$

Note that every non-empty word w in e_0, e_1 can be written as a product of alternating words, and, from the work of Charlton [8], this can be done uniquely, giving a *block decomposition* of and a degree function on words in e_0, e_1.

Definition 3.12. Given a word w in e_0, e_1, define its *block degree* $\deg_{\mathcal{B}}(w)$ to be the number of alternating words in its block decomposition minus one. Equivalently

$$\deg_{\mathcal{B}}(w) = \text{ number of subsequences of } w \text{ of the form } e_ie_i$$

Define the block degree of the empty word to be $\deg_{\mathcal{B}}(\emptyset) = 0$.

Remark 3.13. Note that, unlike depth, the block degree of a word is preserved under the action of the duality operator $\mathrm{D} = RS$, suggesting it may be a more natural degree to assign to the corresponding MZVs.

This induces a filtration on words and hence on multiple zeta values. Note that, for convergent words w, $\deg_{\mathcal{B}}(w) = \deg_{\mathcal{B}}(e_0 w e_1)$, and hence considering endpoints in the corresponding iterated integral is irrelevant. Thus, our definitions are best restricted to convergent words. However, as divergent words will on occasion appear in our cal-cualations, we must choose a convention for such words. We shall initially choose to simply take the "true" block degree of w to be $\deg_{\mathcal{B}}(w)$, regardless of the convergence or divergence of w.

Definition 3.14. Define the block filtration on $\mathcal{H}$, and hence $\mathcal{Z}$, by

$$\mathcal{B}_n\mathcal{H} := \langle \zeta^{\mathfrak{m}}(w) | w \text{ convergent with } \deg_{\mathcal{B}}(w) \leq n \rangle_{\mathbb{Q}}$$

Remark 3.15. Demanding that w be convergent is vital in this definition, or else we have issues such as $\zeta^{\mathfrak{m}}(3) = 0$ in the associated graded: as we have $\zeta^{\mathfrak{m}}(e_0 e_1 e_0) = -2\zeta^{\mathfrak{m}}(e_1 e_0^2)$, we find that $\zeta^{\mathcal{B}}(e_1 e_0^2) = \zeta^{\mathcal{B}}(3) = 0$ in the block grading if we take $\deg_{\mathcal{B}} e_0 e_1 e_0 = 0$. In order to avoid this issue, we must either take the above definition, or define block degree at the level of iterated integrals and account for endpoints.

For example, $\mathcal{B}_0\mathcal{H} = \bigoplus_{n\geq 0} \zeta^{\mathfrak{m}}(\{2\}^n)\mathbb{Q}$. Then, as $\zeta^{\mathfrak{m}}(\{2\}^n) \in \zeta^{\mathfrak{m}}(2)^n\mathbb{Q}$, we have $\mathcal{B}_0\mathcal{Z} \cong \mathbb{Q}[\pi^2]$.

The block filtration is particularly nice for two main reasons: it is easy to determine for the Hoffman basis, and it is preserved by the motivic coaction.

Lemma 3.16 (Brown)**.** *The block filtration induces the level filtration on the subspace spanned by the Hoffman motivic multiple zeta values $\zeta^{\mathfrak{m}}(n_1, \ldots, n_r)$, with $n_i \in \{2, 3\}$, where the level is the number of indices equal to* 3.

Proof. The word corresponding to $(n_1, \ldots, n_r)$, with $n_i \in \{2, 3\}$ of level m has exactly m occurences of the subsequence $e_0 e_0$ and none of $e_1 e_1$. Therefore, it's block degree is exactly $m + 1$. □

As level is motivic, this motivates the following proposition, due to Brown.

Proposition 3.17 (Brown)**.** *Let $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$ denote the de Rham motivic Galois group of the category $\mathcal{MT}(\mathbb{Z})$, and let $U^{dR}_{\mathcal{MT}(\mathbb{Z})}$ denote its unipotent radical. Then $\mathcal{B}_n$ is stable under the action of $G^{dR}_{\mathcal{MT}(\mathbb{Z})}$, and $U^{dR}_{\mathcal{MT}(\mathbb{Z})}$ acts trivially on $gr^{\mathcal{B}}_{\cdot}\mathcal{Z}^{\mathfrak{m}}$. Equivalently*

$$\Delta(\mathcal{B}_n\mathcal{H} \subset \mathcal{O}(U^{dR}_{\mathcal{MT}(\mathbb{Z})}) \otimes \mathcal{B}_{n-1}\mathcal{H}$$

Proof. The motivic coaction factors through D_{2r+1}, and thus it suffices to show that

$$D_{2r+1}\mathcal{B}_k\mathcal{H} \subset \mathcal{O}(U^{dR}_{\mathcal{MT}(\mathbb{Z})}) \otimes \mathcal{B}_{k-1}\mathcal{H}$$

Suppose $a_0 = 0$, $a_{N+1} = 1$, and $a_1 a_2 \ldots a_N$ is convergent of $\mathcal{B}$-degree k. It a can then be written unqiuely as

$$w = v_1 v_2 \ldots v_k$$

of k alternating words $v_i \in A$. Note that, in the formula for D_{2r+1}, all terms with $a_p = a_{p+2r+2}$ vanish. Thus, we can assume $a_p \neq a_{p+2r+2}$, and so every non-zero term on the right hand side is convergent and of total $\mathcal{B}$-degree at most k.Here, we have invoked the following obvious lemma:

Lemma 3.18. *A word w is convergent if and only if it begins in e_1 and*

$$deg_{\mathcal{B}}(w) - |w| \equiv 0 \text{ (mod 2)}$$

where $|w|$ denotes the length of w.

We can furthermore conclude that

$$a_p a_{p+1} \dots a_{p+2r+2} \notin A$$

as any alternating word of odd length must begin and end with the same letter. Thus a_p and a_{p+2r+2} are not letters in the same word v_i, implying that the right hand tensor factor of each term in the coproduct have $\mathcal{B}$-degree strictly less than k. □

We get the following neat corollary, further emphasizing the block filtration as *the* natural, filtration on $\mathcal{H}$.

Corollary 3.19 (Brown)**.** *The block filtration on $\mathcal{H}$ is precisely the coradical filtration.*

3.3 Block graded relations

As the block filtration is motivic, we would expect that, upon taking the associated graded, we obtain fairly simple relations. Indeed, by simply doing the calculations, we find that, up to weight 5, there are no non trivial relations other than duality among convergent block graded multiple zeta values.

In light of lemma 3.16 and the main theorem of [4], one has the following theorem:

Theorem 3.20 (Brown)**.** *Every element in $\mathcal{B}_n\mathcal{H}$ of weight N can be written uniquely as a $\mathbb{Q}$-linear combination of motivic Hoffman elements of weight N and level at most n.*

This would lead us to expect that we get the following dimensions in the associated graded:

$$\sum_{n=0}^{\infty} \dim \operatorname{gr}_m^{\mathcal{B}} \mathcal{H}_n s^m t^n = \frac{1}{1 - t^2 - st^3}$$

Precisely, in the associated graded, we have exactly the following relations among nonzero MZVs and we would like these to be the only relations. Any convergent zeta values not appearing in the table become zero in the block grading.

Weight	1	2	3	4	5
	$\varnothing$	$\zeta^{\mathcal{B}}(2)$	$\zeta^{\mathcal{B}}(3) = \zeta^{\mathcal{B}}(1,2)$	$\zeta^{\mathcal{B}}(2,2)$	$\zeta^{\mathcal{B}}(2,3) = \zeta^{\mathcal{B}}(1,2,2)$ $\zeta^{\mathcal{B}}(3,2) = \zeta^{\mathcal{B}}(2,1,2)$

Remark 3.21. We denote by $\zeta^{\mathcal{B}}(w)$ the projection of $\zeta^{\mathfrak{m}}(w)$ into $\mathrm{gr}^{\mathcal{B}}\mathcal{H}$.

Remark 3.22. Note the $\zeta^{\mathcal{B}}(N) = 0$ for all $N > 3$, as $\deg_{\mathcal{B}}(\zeta^{\mathfrak{m}}(N)) = n-1$, but, writing $\zeta^{\mathfrak{m}}(N)$ in the Hoffman basis, we have $\zeta^{\mathfrak{m}}(N) \in \mathcal{B}_{\frac{N}{3}}\mathcal{H}$.

However, if we were to have allowed divergent words in our definition, we would obtain more relations and in fact lose linear independence of the Hoffman basis.

Example 3.23. As $2\zeta^{\mathfrak{m}}(2,3) + 2\zeta^{\mathfrak{m}}(3,2) = \zeta^{\mathfrak{m}}(2,2,1)$, in the block graded we get $\zeta^{\mathcal{B}}(2,3) + \zeta^{\mathcal{B}}(3,2) = 0$. Thus they cannot be linearly independent. Indeed, we will always find that the Hoffman elements are not linearly independent in odd weight in the associated graded, as we can always write $\zeta^{\mathfrak{m}}(2,\ldots,2,1)$ as a $\mathbb{Q}$-linear combination of Hoffman elements, and $\deg_{\mathcal{B}}(e_1e_0\ldots e_1) = 0$, for all $N \geq 3$.

Thus, in our calculations, we no longer have that the Hoffman basis for motivic multiple zeta values is a basis. While this doesn't severely impact our ability to perform calculations using the double shuffle relations, we are hampered in our use of the motivic coaction due to the reliance on renormalisation. This is something we hope to overcome, as $\zeta(N) = 0$ in the block grading, for all $N > 3$. This means that Brown's algorithm for decomposition of MZVs into a basis [5] becomes exact in the block grading.

Using that the Hoffman basis for motivic multiple zeta values is a spanning set, we can explicitly compute the parts of the infinitesimal motivic coaction.

Lemma 3.24 (K.)**.** *If we define the block filtration without change for divergent words w, D_3 acts trivially on $gr^{\mathcal{B}}\mathcal{H}$.*

Proof. It suffices to show this holds for the Hoffman basis for motivic multiple zeta values. Suppose $I^{\mathfrak{m}}(0;1010\ldots1010;1)$ represents an element of the Hoffman basis. The binary sequence then consists of alternating 0s and 1s, with the occasional 00. Thus, $\mathrm{D}_3 I^{\mathfrak{m}}(0;1010\ldots1010;1)$ consists of a sum over terms whose left tensor factor is of weight 3. If we allow divergent words, all weight three elements vanish. $\square$

3.4 Block grading with divergent words

If, instead of taking the block degree as we have defined it, we took $\deg_{\mathcal{B}}{}^*(w) := \deg_{\mathcal{B}}(e_0we_1)$, it is possible that the issues associated with divergent words could be resolved. For example $\deg_{\mathcal{B}}{}^*(e_0e_1e_0) = 1 = \deg_{\mathcal{B}}{}^*(e_1e_0^2)$, and so we could allow $\zeta^{\mathfrak{m}}(e_0e_1e_0)$, without $\zeta^{\mathfrak{m}}(3) = 0$ in the associated graded. This is a possibility not yet fully explored.

It does seem to resolve many of our issues though: for example $\deg_{\mathcal{B}}{}^*(\zeta^{\mathfrak{m}}(2,\ldots,2,1) = 1$, and we have

$$\begin{aligned}
\zeta^{\mathfrak{m}}(2,\ldots,2,1) &= I^{\mathfrak{m}}(0;1,0,1,\ldots,0,1;1) \\
&= -I^{\mathfrak{m}}(0;0,1,0,\ldots,1,0;1) \text{ (Apply reversal of paths and functoriality)} \\
&= \sum_{i_1+\cdots+i_r} \binom{i_1+1}{i_1}\cdots\binom{i_r+1}{i_r} I^{\mathfrak{m}}(0;1,\{0\}^{i_1+1},\ldots,1,\{0\}^{i_r+1};1) \text{ (Shuffle regularisation)} \\
&= 2\sum_{i=0}^{r-1} \zeta^{\mathfrak{m}}(\{2\}^i,3,\{2\}^{r-1-i})
\end{aligned}$$

When taking the block graded version of this, $\zeta^{\mathcal{B}}(2,\ldots,2,1)$ does not get quotiented out, preserving linear independence of these Hoffman elements. Thus we believe this to be the correct formulation. Indeed, expression of divergent MZVs in terms of convergent MZVs via shuffle regularisation preserves this definition of block degree.

Proposition 3.25 (K.). *$deg_{\mathcal{B}}{}^*(w) = N$ implies $\zeta^{\mathfrak{m}}(w) \in \mathcal{B}_n\mathcal{H}$*

Proof. As $\deg_{\mathcal{B}}{}^*(w) = \deg_{\mathcal{B}}(w)$ for convergent words w, we need only consider divergent words. Furthermore, duality allows us to reduce our analysis to the case were $w = e_0u$ for some word u. We first consider the case where $w = e_0ve_0$ for some v.

Suppose $w = e_0^k e_1 e_0^{n_1} \ldots e_1 e_0^{n_r}$. Shuffle regularisation of the corresponding iterated integral gives

$$\begin{aligned}&(-1)^k I^{\mathfrak{m}}(0; \{0\}^k, 1, \{0\}^{n_1}, \ldots, 1, \{0\}^{n_r}; 1) = \\ &\sum_{i_1+\cdots+i_r=k} \binom{n_1+i_1}{i_1} \cdots \binom{n_r+i_r}{i_r} I^{\mathfrak{m}}(0; 1, \{0\}^{n_1+i_1}, \ldots, 1, \{0\}^{n_r+i_r}; 1)\end{aligned}$$

Each term on the right hand side arises from inserting one of the first k 0's into the sequence at some point after the first 1. Each inserted 0 either increases the number of repetitions of 0 in the sequence by 1, or decreases the number of repetitions of 1 by 1. So for any given insertion of 0's, we can increase the block degree of $(1, \{0\}^{n_1}, \ldots, 1, \{0\}^{n_r})$ by at most k. Thus, the adjusted $\mathcal{B}$-degree of every term on the right hand side is at most $\deg_{\mathcal{B}}(1, \{0\}^{n_1}, \ldots, 1, \{0\}^{n_r}) + k = \deg_{\mathcal{B}}{}^*(w)$. Thus the result is shown for words starting and ending with e_0.

For words $w = e_0ve_1$, we have $\deg_{\mathcal{B}}{}^*(w) = \deg_{\mathcal{B}}(w) + 2$. Applying shuffle regularisation to the corresponding iterated integral, we can split the sum into two parts:

$$\begin{aligned}&(-1)^k I^{\mathfrak{m}}(0; \{0\}^k, 1, \{0\}^{n_1}, \ldots, 1; 1) = \\ &\sum_{i_1+\cdots+i_r=k, i_r\geq 1} \binom{n_1+i_1}{i_1} \cdots \binom{n_r+i_r}{i_r} I^{\mathfrak{m}}(0; 1, \{0\}^{n_1+i_1}, \ldots, 1, \{0\}^{n_{r_1}+i_{r-1}}, 1, \{0\}^{i_r}; 1) + \\ &\sum_{i_1+\cdots+i_{r-1}=k} \binom{n_1+i_1}{i_1} \cdots \binom{n_{r-1}+i_{r-1}}{i_{r-1}} I^{\mathfrak{m}}(0; 1, \{0\}^{n_1+i_1}, \ldots, 1, \{0\}^{n_{r_1}+i_{r-1}}, 1; 1)\end{aligned}$$

As argued before, all terms in the first line have adjusted $\mathcal{B}$-degree at most

$$\deg_{\mathcal{B}}(1, \{0\}^{n_1+i_1}, \ldots, 1, \{0\}^{n_{r_1}+i_{r-1}}, 1) + k - 1 < \deg_{\mathcal{B}}{}^*(w)$$

Terms in the second line are still divergent, with adjusted $\mathcal{B}$-degree at most $\deg_{\mathcal{B}}{}^*(w)$. Applying duality and shuffle regularisation once more, we see that $\deg_{\mathcal{B}}{}^*(w)$ is an upper bound for the $\mathcal{B}$-degree of all convergent terms on the right hand side, proving the claim. $\square$

This proof also highlights a few interesting facts about shuffle regularisation in the associated graded.

Corollary 3.26 (K.). *For a word w beginning with e_0, all terms $\zeta^{\mathcal{B}}(n_1, \dots, n_r)$ appearing on the right hand side of the equality $\zeta^{\mathcal{B}}(w) = \dots$ have that $\#\{i|n_i = 1\} =$ number of e_1e_1 subsequences in w as a common constant.*

Proof. If we have a term on the right hand side corresponding the iterated integral arising from insertion of 0's between two adjacent 1's, it will have strictly lower block degree, as $\deg_{\mathcal{B}}(e_0^{i+1}e_1e_1) = i+1$, but $\deg_{\mathcal{B}}(e_0e_1e_0^ie_1) = i-1$, so we "lose" two repetitions. Thus, terms where adjacent 1's are separated drop out in the associated graded. □

Corollary 3.27 (K.). *In the shuffle regularisation of $\zeta^{\mathcal{B}}(n_1, \dots, n_{r-1}, 1)$, all terms $\zeta^{\mathcal{B}}(m_1, \dots, m_k)$ have $\#\{i|m_i = 1\}$ as a common constant, which is equal to $n_1 + \cdots + n_{r-1} + 1 - 2r$.*

Extending our table of relations from the previous section to include relations featuring divergent zeta values, we find the following, where we again omit any elements equal to 0:

Weight	1	2	3	4
	$\varnothing$	$\zeta^{\mathcal{B}}(e_0e_1) = -\zeta^{\mathcal{B}}(2)$	$\zeta^{\mathcal{B}}(e_0e_1e_0) = -2\zeta^{\mathcal{B}}(3)$ $\zeta^{\mathcal{B}}(2,1) = 2\zeta^{\mathcal{B}}(3)$	$\zeta^{\mathcal{B}}(e+0^2e_1e_0) = 3\zeta^{\mathcal{B}}(4)$ $\zeta^{\mathcal{B}}(e_0e_1e_0^2) = -3\zeta^{\mathcal{B}}(4)$ $\zeta^{\mathcal{B}}(e_0e_1^2e_0) = -2\zeta^{\mathcal{B}}(1,3)$ $\zeta^{\mathcal{B}}(3,1) = -2\zeta^{\mathcal{B}}(1,3)$ $\zeta^{\mathcal{B}}(e_0e_1e_0e_1) = 4\zeta^{\mathcal{B}}(1,3)$ $\zeta^{\mathcal{B}}(1,2,1) = -3\zeta^{\mathcal{B}}(4)$ $\zeta^{\mathcal{B}}(2,1,1) = 3\zeta^{\mathcal{B}}(4)$

We have omitted the weight 5 relations for sake of brevity. We find simply that every value is 0, or a linear combination of $\zeta^{\mathcal{B}}(2,3)$ and $\zeta^{\mathcal{B}}(3,2)$.

Note that, in this formulation, we have $\zeta^{\mathcal{B}}(e_0e_1e_0) = -2\zeta^{\mathcal{B}}(3)$ is non-zero, so our proof that D_3 is trivial on all elements of $\mathrm{gr}^{\mathcal{B}}\mathcal{H}$ no longer holds, as weight three is now non-zero. We will instead move from $\mathcal{H}$ to $\mathcal{A} = \mathcal{H}/\zeta^{\mathfrak{m}}(2)$, in which Δ is a true coproduct rather than a coaction. Much work is needed to be done here, but a successful theory of block graded renormalised MZVs has the potential to be quite powerful. And it appears that this is the correct choice of extension of the block filtration to divergent MZVs, as it is motivic. We first show the following.

Proposition 3.28 (K.). *Defining $\mathcal{B}_n\mathcal{H} := \langle \zeta^{\mathfrak{m}}(w) | deg_{\mathcal{B}}{}^*(w) \leq n\rangle_{\mathbb{Q}}$, this extended block filtration is motivic:*

$$\Delta \mathcal{B}_n\mathcal{H} \subset \sum_{k=1}^{n-1} \mathcal{B}_k\mathcal{H} \otimes \mathcal{B}_{n-k}\mathcal{H}$$

Proof. Consider $I^{\mathfrak{m}}(0; w; 1)$, w a word in $\{0,1\}$ such that $\deg_{\mathcal{B}}{}^*(w) \leq n$. We wish to show that every term of $\Delta I^{\mathfrak{m}}(0; w; 1)$ is in $\mathcal{B}_k\mathcal{H} \otimes \mathcal{B}_{n-k}\mathcal{H}$, for some $1 \leq k < n$. Proposition 3.17 shows this for w convergent, so we need only consider the case of divergent w. Furthermore, as duality preserves block degree, we may assume

$$I^{\mathfrak{m}}(0;w;1) = I^{\mathfrak{m}}(0;\{0\}^m v_1,\dots,v_r;1)$$

where v_i are alternating.

We once again consider the infinitesimal actions D_{2a+1}. All non-zero terms in $D_{2a+1}(I^{\mathfrak{m}}(0;\{0\}^m v_1,\dots,v_r;1)$ will be of the form

$$I^{\mathfrak{a}}(0;\{0\}^s u;1)\otimes I^{\mathfrak{m}}(0;\{0\}^t 1v;1) \text{ for } s+t=m\ s\geq 1$$
$$\text{or}$$
$$I^{\mathfrak{a}}(0;y;1)\otimes I^{\mathfrak{m}}(0;\{0\}^m,xz;1)$$

where $w=\{0\}^m u1v$ in the first case and $w=\{0\}^m xyz$ in the latter. In the second case, one can see that the result holds by following the arguments of Proposition 3.17. In the first case, we must do slightly more work.

Note that

$$\deg_{\mathcal{B}}{}^*(w) = \deg_{\mathcal{B}}(\{0\}^{m+1}u1v1) = m + \deg_{\mathcal{B}}(u1v1)$$

and that

$$\deg_{\mathcal{B}}{}^*(\{0\}^s u) = s + \deg_{\mathcal{B}}(w1)$$
$$\deg_{\mathcal{B}}{}^*(\{0\}^t 1v) = t + \deg_{\mathcal{B}}(1v1)$$

Thus $\deg_{\mathcal{B}}{}^*(\{0\}^s u) + \deg_{\mathcal{B}}{}^*(\{0\}^t 1v) = m + \deg_{\mathcal{B}}(w1) + \deg_{\mathcal{B}}(1v1)$. We see that

$$\deg_{\mathcal{B}}(ua) + \deg_{\mathcal{B}}(av) = \deg_{\mathcal{B}}(uav)$$

for u,v words in $\{0,1\}$, and $a\in\{0,1\}$, as this overlapped concatenation can neither create nor destroy subsequences of the form ii. Finally, we note that, if $\deg_{\mathcal{B}}{}^*(\{0\}^s u)=0$, we must have $s=0$, which puts us into the second case. Thus, the extended block filtration is motivic. $\square$

We can in fact show the following, stronger, statement quite easily.

Theorem 3.29 (K.). *The motivic coproduct is graded for the extended block filtration:*

$$\Delta gr_n^{\mathcal{B}}\mathcal{A} \subset \bigoplus_{k=1}^{n} -1 gr_k^{\mathcal{B}}\mathcal{A}\otimes gr_{n-k}^{\mathcal{B}}\mathcal{A}$$

Proof. Consider $I^{\mathfrak{a}}(0;w;1)$, w a word in $\{0,1\}$ such that $\deg_{\mathcal{B}}{}^*(w)=n$. Then we can decompose $0w1=b_1b_2\dots b_{n+1}$ into alternating blocks, and consider the action of D_{2n+1} on $I^{\mathfrak{a}}(b_1\dots b_{n+1})$. All terms in $D_{2n+1}I^{\mathfrak{a}}(b_1\dots b_{n+1})$ will be of the form

$$I^{\mathfrak{a}}(x;b_i''b_{i+1}\dots b_{i+j}';y)\otimes I^{\mathfrak{a}}(b_1\dots b_{i-1}b_i'xyb_{i+j}''b_{i+j+1}\dots b_{n+1})$$

for some $1 \leq i \leq n+1$, where $b_i = b_i' x b_i''$, $b_{i+j} = b_{i+j}' y b_{i+j}''$. For the left hand term to be non-zero, we must have $x \neq y$, and so we see

$$\deg_{\mathcal{B}}(x b_i'' b_{i+1} \dots b_{i+j}' y) = j$$
$$\deg_{\mathcal{B}}(b_1 \dots b_i' x y b_{i+j}'' \dots b_{n+1} = n - j$$

by counting the blocks. Then, as we included the endpoints in our calculations, we get that the total extended block degree of any term in the coproduct is n. $\square$

Knowing that the motivic coproduct is block graded, we can then use it to describe relations among block graded MZVs. Define

$$\mathcal{A}^{\mathcal{B}} := \bigoplus_{n=1}^{\infty} \mathrm{gr}_n^{\mathcal{B}} \mathcal{A}$$

and let $\mathcal{L} := \mathcal{A}_{>0}^{\mathcal{B}} / \mathcal{A}_{>0}^{\mathcal{B}} \mathcal{A}_{>0}^{\mathcal{B}}$ be the Lie coalgebra of indecomposables. Its dual, which we shall denote by $\mathfrak{bg}$, encodes all relations among block graded MZVs modulo $\zeta^{\mathfrak{m}}(2)$ and products. We expect it to be Lie algebra with a unique generator in every odd weight, similar to $\mathfrak{ls}$, however we expect here that it will be a free Lie algebra.

As the coproduct on $\mathcal{A}^{\mathcal{B}}$ is precisely the motivic coproduct, the dual product on $\mathcal{U}\mathfrak{bg}$ will be the block-graded Ihara product.

Lemma 3.30 (K.)**.** *The block graded Ihara product is given by*

$$\begin{aligned} w \circ^{\mathcal{B}} e_0^{n_0} e_1 \dots e_1 e_0^{n_k} &= \sum_{i=0}^{k} (1 - \delta_{w_1, e_0} \delta_{n_i, 0}) e_0^{n_0} e_1 \dots e_0^{n_i} w e_1 \dots e_1 e_0^{n_k} \\ &+ \sum_{i=0}^{k-1} (1 - \delta_{w_1, e_0} \delta_{n_{i+1}, 0}) e_0^{n_0} e_1 \dots e_0^{n_i} e_1 w e_0^{n_{i+1}} \dots e_1 e_0^{n_k} \end{aligned}$$

where $w = w_1 \dots w_r$, $w^* = (-1)^r w_r \dots w_1$, and $\delta_{a,b} = 1$ if $a = b$ and 0 otherwise.

Proof. Expanding the recursive definition of the Ihara product we get

$$w \circ e_0^{n_0} e_1 \dots e_1 e_0^{n_k} = \sum_{i=0}^{k} e_0^{n_0} e_1 \dots e_0^{n_i} w e_1 \dots e_1 e_0^{n_k} + \sum_{i=0}^{k-1} e_0^{n_0} e_1 \dots e_0^{n_i} e_1 w e_0^{n_{i+1}} \dots e_1 e_0^{n_k}$$

in which every term is of the form $e_0^{n_0} e_1 \dots e_0^{n_i} w e_1 \dots e_1 e_0^{n_k}$ or $e_0^{n_0} e_1 \dots e_0^{n_i} e_1 w e_0^{n_{i+1}} \dots e_1 e_0^{n_k}$.

Considering the first form, and assuming $n_i \neq 0$, we have

$$\begin{aligned} \deg_{\mathcal{B}}(e_0 \cdot e_0^{n_0} e_1 \dots e_0^{n_i} w e_1 \dots e_1 e_0^{n_k} \cdot e_1) &= \deg_{\mathcal{B}}(e_0 \cdot e_0^{n_0} e_1 \dots e_0^{n_i}) + \deg_{\mathcal{B}}(e_0 w e_1) + \deg_{\mathcal{B}}(e_1 \dots e_1 e_0^{n_k} \cdot e_1) \\ &= \deg_{\mathcal{B}}(e_0 w e_1) + \deg_{\mathcal{B}}(e_0 \cdot e_0^{n_0} e_1 \dots e_0^{n_i} e_1 \dots e_1 e_0^{n_k} \cdot e_1) \end{aligned}$$

using $\deg_{\mathcal{B}}(uxv) = \deg_{\mathcal{B}}(ux) + \deg_{\mathcal{B}}(xv)$ for a letter x. Thus

$$\deg_{\mathcal{B}}{}^*(e_0 \cdot e_0^{n_0} e_1 \dots e_0^{n_i} w e_1 \dots e_1 e_0^{n_k} \cdot e_1) = \deg_{\mathcal{B}}{}^*(w) + \deg_{\mathcal{B}}{}^*(e_0^{n_0} e_1 \dots e_0^{n_i} e_1 \dots e_1 e_0^{n_k})$$

Now, if $n_i = 0$, we instead get

$$\begin{aligned}\deg_{\mathcal{B}}(e_0 \cdot e_0^{n_0} e_1 \dots e_1 w e_1 \dots e_1 e_0^{n_k} \cdot e_1) &= \deg_{\mathcal{B}}(e_0 \cdot e_0^{n_0} e_1 \dots e_1) + \deg_{\mathcal{B}}(e_1 w e_1) + \deg_{\mathcal{B}}(e_1 \dots e_1 e_0^{n_k} \cdot e_1) \\ &= \deg_{\mathcal{B}}(e_1 w e_1) + \deg_{\mathcal{B}}(e_0 \cdot e_0^{n_0} e_1 \dots e_1 e_1 \dots e_1 e_0^{n_k} \cdot e_1) - 1\end{aligned}$$

Then

$$\deg_{\mathcal{B}}(e_1 w e_1) = \begin{cases} \deg_{\mathcal{B}}(e_0 w e_1) + 1 & \text{if } w_1 = e_1 \\ \deg_{\mathcal{B}}(e_0 w e_1) - 1 & \text{if } w_1 = e_0 \end{cases}$$

Thus the extended degree of such terms is $\deg_{\mathcal{B}}{}^*(w) + \deg_{\mathcal{B}}{}^*(e_0^{n_0} e_1 \dots e_0^{n_i} e_1 \dots e_1 e_0^{n_k})$ unless $w_1 = e_0$ and $n_i = 0$. Hence, we can block grade by introducing these $(1 - \delta_{w_1, e_0} \delta_{n_i, 0})$ factors. Similar analysis gives the δ factors in the second sum.

□

As generators of $\mathfrak{bg}$, we choose generating series of weight $2k+1$, block degree 1 Hoffman elements.

Definition 3.31. Define p_{2k+1} as the block grading of one of the following, after rescaling by $1/\zeta^{\mathfrak{m}}(2k+1)$:

$$p_{2k+1} := \sum_{i=0}^{k-1} \zeta^{\mathfrak{m}}(\{2\}^i, 3, \{2\}^{k-1-i}) (e_1 e_0)^i e_1 e_0^2 (e_1 e_0)^{k-1-i}$$

$$p_{2k+1} := x_1 \dots x_k \sum_{i=1}^{k} \zeta^{\mathfrak{m}}(\{2\}^i, 3, \{2\}^{k-1-i}) x_{i+1}$$

$$p_{2k+1} := \sum_{i=0}^{k-1} \zeta^{\mathfrak{m}}(\{2\}^i, 3, \{2\}^{k-1-i}) x^{2i+2} y^{2k-2i-1}$$

Note that the first two definitions are equivalent by our standard transition between commutative and noncommutative polynomials. The third is more like the work of Zagier [33]. Indeed, we can use his work to express the third definition more concisely.

Lemma 3.32 (K.)**.**

$$p_{2k+1} = (-1)^k \left[y((x+y)^{2k} + (x-y)^{2k} - 2y^{2k}) - (1 - \frac{1}{2^{2k}}) x((x+y)^{2k} - (x-y)^{2k}) \right]$$

Proof. From theorem 1 of [33], we have that, modulo $\zeta^{\mathfrak{m}}(2)$

$$\zeta^{\mathfrak{m}}(\{2\}^a, 3, \{2\}^b) = 2 \times (-1)^{a+b+1} \left[\binom{2a+2b+2}{2a+2} - (1 - \frac{1}{2^{2a+2b+2}} \binom{2a+2b+2}{2b+1} \right] \zeta^{\mathfrak{m}}(2a+2b+3)$$

Filling this into our definition of p_{2k+1} and simplifying, we get the desired polynomial.

□

4 Further Work and Conjectures

4.1 Some partial results on duality

As it is conjectured that the double shuffle equations describe all non-trivial relations among multiple zeta values, in particular the duality arising from symmetry of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, we considered various methods of deriving duality as a consequence of the double shuffle relations. Some progress has been made towards this [23][24], but is restricted to sums of zeta values or low depths, or invokes the so-called 'derivation' relations [22] as a stepping stone.

Our approach, while ultimately incomplete, instead considers elements of $\mathfrak{dmr}_0$, and attempts to show duality holds here. We first observe that

$$\mathbb{Q}\langle a, b\rangle = \mathbb{Q}^{\mathrm{D}}\langle a, b\rangle \oplus \mathbb{Q}^{-\mathrm{D}}\langle a, b\rangle$$

where

$$\mathbb{Q}^{\mathrm{D}}\langle a, b\rangle := \{\phi \in \mathbb{Q}\langle a, b\rangle | \mathrm{D}\phi = \phi\}$$
$$\mathbb{Q}^{-\mathrm{D}}\langle a, b\rangle := \{\phi \in \mathbb{Q}\langle a, b\rangle | \mathrm{D}\phi = -\phi\}$$

If we assume $\mathrm{D}\mathfrak{dmr}_0 \subset \mathfrak{dmr}_0$, then $\mathfrak{dmr}_0$ splits similarly. Indeed, as the double shuffle equations are motivic, one expects this to be the case [30]. Hence, it would suffice to show that no non-zero $\phi \in \mathfrak{dmr}_0$ satisfied $\mathrm{D}\phi = -\phi$. Suppose such a ϕ exists: we may suppose, without loss of generality, that it is homogeneous of weight N.

If $N = 2k$, the depth k component of ϕ must be 0. We can similarly show that, for $N = 2k + 1$, the depth k component of ϕ must be zero. Hence the problem of duality is reduced to the existence of solutions to the linearised double shuffle equations of high depth relative to weight.

Here, by applying techniques similar to those of [21], we found limited success, with certain parity constraints being necessary, invoking the depth-parity theorem as an initial step. We will loosely sketch the idea, but will not fill in the details, as much of the proof is dependent on choice of n.

Sketch. Start by defining a right action of $\mathrm{GL}_n(\mathbb{Q})$ on $\mathbb{Q}[x_1, \dots, x_n]$ by

$$(f|_S)(x) := f(xS^{-1})$$

Next define $R := J - (n-1)I$, where J is the matrix with 1 in each entry. Letting $g := f|_R$, we note that f solving the linearised double shuffle equations is equivalent to g solving slightly modified versions. In particular, the equations solved by g imply that g is invariant under the action of two subgroups $W, W' < \mathrm{GL}_n(\mathbb{Q})$. If we can show that $\langle W, W'\rangle$ contains a subgroup Γ of finite index in $\mathrm{GL}_n(\mathbb{Q})$, we can apply [21] Proposition 8 to conclude that g, and hence f is constant. From here, it is easy to conclude that f is 0.

There is also potential to utilise the motivic coaction, and possibly Brown's algorithm for decomposition of motivic MZVs into a given basis [4], to prove the duality relation.

Lemma 4.1 (K.). *The duality operator D commutes with the infinitesimal coaction operators D_{2r+1}.*

Proof.

$$D_r \mathrm{D} I^{\mathfrak{m}}(0; a_1, \ldots, a_n; 1) = D_r (-1)^n I^{\mathfrak{m}}(0; 1-a_n, \ldots, 1-a_1; 1)$$
$$= \sum_{p=0}^{n-r} (-1)^n I^{\mathfrak{a}}(1-a_{n-p}; 1-a_{n-p-1}, \ldots, 1-a_{n-p-r}; 1-a_{n-p-r-1})$$
$$\otimes I^{\mathfrak{m}}(0; 1-a_n, \ldots, 1-a_{n-p}, 1-a_{n-p-r-1}, \ldots, 1-a_1; 1)$$
$$= \mathrm{D} \otimes \mathrm{D} \sum_{p=0}^{n-r} I^{\mathfrak{a}}(1-a_{n-p}; a_{n-p-r}, \ldots, a_{n-p-1}; 1-a_{n-p-r-1}) \otimes I^{\mathfrak{m}}(0; a_1, \ldots, a_{n-p-r-1}, a_{n-p}, \ldots, a_n; 1)$$
$$= \mathrm{D} \otimes \mathrm{D} \sum_{p=0}^{n-r} I^{\mathfrak{a}}(1-a_{p+r+1}; a_{p+1}, \ldots, a_{p+r}; 1-a_p) \otimes I^{\mathfrak{m}}(0; a_1, \ldots, a_p, a_{p+r+1}, \ldots, a_n; 1)$$

Then noting that $a_p = a_{p+r+1} \Leftrightarrow 1-a_p = 1-a_{p+r+1}$, the only non-zero terms in $D_r I^{\mathfrak{m}}(0; a_1, \ldots, a_n; 1)$ or $D_r \mathrm{D} I^{\mathfrak{m}}(0; a_1, \ldots, a_n; 1)$ are those with $a_p = 1 - a_{p+r+1}$. Thus we have

$$D_r \mathrm{D} I^{\mathfrak{m}}(0; a_1, \ldots, a_n; 1) = \mathrm{D} \otimes \mathrm{D} D_r I^{\mathfrak{m}}(0; a_1, \ldots, a_n; 1)$$

□

Corollary 4.2. *$D\zeta^{\mathfrak{m}}(N) = c\zeta^{\mathfrak{m}}(N)$ for some $c \in \mathbb{Q}$.*

Proof. Suppose we have some $\sigma \in \mathcal{H}_N$ such that $D_{<N}\sigma = 0$. Such a σ always exists as a consequence of the double shuffle relations. Thus $\sigma = \alpha\zeta^{\mathfrak{m}}(N)$.Furthermore, we can choose σ so that $\alpha \neq 0$. D commutes with $\mathrm{D}_{<N}$ and so $D_{<N}\mathrm{D}\sigma = 0$. Hence we have

$$\alpha \mathrm{D} \zeta^{\mathfrak{m}}(N) = \mathrm{D}\sigma = \beta\zeta^{\mathfrak{m}}(N)$$

for some $\beta \in \mathbb{Q}$. The result follows. □

However, this method only serves to restrict the dimension of the vector spaces of weight N. Fixing the coefficient requires more machinery.

4.2 On the coefficients of a rational associator

As the double shuffle equations are defined over the integers, we can consider their reduction modulo primes to gain some information about the complexity of its coefficients.Continuing our slight abuse of notation, we shall refer to every depth of a solution as Φ, as the depth can be inferred from the number of variables.

Theorem 4.3 (K.). *There are no non-trivial solutions to the shuffle equation modulo p, p prime.*

Proof. Suppose Φ sovles the shuffle equations. Then, for any $k \geq 1$, we have

$$\begin{aligned}
&\Phi(x_{1,1}, x_{1,2}, \ldots, x_{1,k})\Phi(x_{2,1}, x_{2,2}, \ldots, x_{2,k}) \cdots \Phi(x_{p,1}, x_{p,2}, \ldots, x_{p,k}) \\
&\quad = \Phi^{\natural}(\boldsymbol{x}_{1,1} \ldots \boldsymbol{x}_{1,k} \sqcup\!\sqcup \boldsymbol{x}_{2,1} \ldots \boldsymbol{x}_{2,k} \sqcup\!\sqcup \cdots \sqcup\!\sqcup \boldsymbol{x}_{p,1} \ldots \boldsymbol{x}_{p,k})
\end{aligned}$$

where $\Phi^{\natural}$ is as defined previously.

The right hand side will split as a sum as follows

$$\sum_{i=1}^{p} \Phi^{\natural}(\boldsymbol{x}_{i,1}(\boldsymbol{x}_{1,1} \ldots \boldsymbol{x}_{1,k} \sqcup\!\sqcup \cdots \sqcup\!\sqcup \boldsymbol{x}_{i,2} \ldots \boldsymbol{x}_{2,k} \sqcup\!\sqcup \cdots \sqcup\!\sqcup \boldsymbol{x}_{p,1} \ldots \boldsymbol{x}_{p,k}))$$

so upon setting $x_{1,j} = x_{2,j} = \cdots = x_{p,j} = x_j$ for each $1 \leq j \leq k$, we find

$$\begin{aligned}
\Phi(x_1, \ldots, x_k)^p &= \sum_{i=1}^{p} \Phi^{\natural}(\boldsymbol{x}_1(\boldsymbol{x}_1 \ldots \boldsymbol{x}_k \sqcup\!\sqcup \cdots \sqcup\!\sqcup \boldsymbol{x}_2 \ldots \boldsymbol{x}_k \sqcup\!\sqcup \cdots \sqcup\!\sqcup \boldsymbol{x}_1 \ldots \boldsymbol{x}_k)) \\
&= p\Phi^{\natural}(\boldsymbol{x}_1(\boldsymbol{x}_2 \ldots \boldsymbol{x}_k \sqcup\!\sqcup \boldsymbol{x}_1 \ldots \boldsymbol{x}_k \sqcup\!\sqcup \cdots \sqcup\!\sqcup \boldsymbol{x}_1 \ldots \boldsymbol{x}_k))
\end{aligned}$$

as the shuffle product is commutative. Thus, we have

$$\Phi(x_1, \ldots, x_k)^p \equiv 0 \bmod p$$

and hence

$$\Phi(x_1, \ldots, x_k) \equiv 0 \bmod p$$

for every $k \geq 1$. $\square$

Corollary 4.4. *There are no non-trivial integer solutions to the shuffle equation.*

Proof. By the above theorem, if an integer solution exists, the coefficients of all terms of positive degree must be divisible by p, for every prime p. Clearly this is impossible unless all terms of positive degree vanish. $\square$

Corollary 4.5. *In any Φ coming from a rational λ-associator, $\lambda \neq 0$, every prime must appear in the denominator of a coefficient of $\Phi(x_1, \ldots, x_k)$ for some $k \geq 1$. That is to say, the denominators of coefficients are, in some sense, arbitrarily complicated.*

Proof. Suppose otherwise: that for some prime p, every coefficient in Φ is an element of $\mathbb{Z}_p$. As the associator equations imply the shuffle equation, the above argument still holds, and so we get that Φ is trivial mod p. But, it is known that the coefficient of x in $\Phi(x)$ must be $\frac{\lambda^2}{24}$ [13]. Thus, Φ cannot be trivial mod p for any $p > 2$, and since $2|24$, the result follows. $\square$

We believe these ideas could be further refined to give more precise results on the growth of coefficients, however, as this is not in line with our current goals, it shall remain an interesting observation.

4.3 Relations and obstructions from period polynomials

One of the challenges in defining canonical σ elements, and in working with $\mathfrak{ls}$ is the existence of relations between σ elements in low depth, such as Ihara's relation

$$3\{\sigma_5, \sigma_7\} = \{\sigma_3, \sigma_9\} \text{ modulo depths } \geq 4$$

However, we can explicitly describe all quadratic relations, as they all arise from period polynomials [17], [26].

Our map $\rho : \mathbb{Q}\langle a, b\rangle \to \bigoplus_{n=1}^{\infty} \mathbb{Q}[y_0, \ldots, y_n]$ descends to a map

$$\bar{\rho} : \mathfrak{ls} \to \bigoplus_{n=1}^{\infty} \mathbb{Q}[y_0, \ldots, y_n] \to \bigoplus_{n=1}^{\infty} \mathbb{Q}[x_1, \ldots, x_n]$$

The Ihara bracket gives a map

$$\{\cdot, \cdot\} : \mathfrak{ls}_1 \wedge \mathfrak{ls}_1 \to \mathfrak{ls}_2$$

which on application of $\bar{\rho}$ gives a map

$$D_1 \wedge D_1 \to D_2$$

where D_i is the $\mathbb{Q}$-vector space of even polynomials in i variables. We find that $D_1 \wedge D_1$ is isomorphic to the space of antisymmetric even polynomials $p(x_1, x_2)$. The image of $p(x_1, x_2)$ under the induced map is

$$p(x_1, x_2) + p(x_2 - x_1, -x_1) + p(-x_2, x_1 - x_2)$$

Recalling Definition 2.37, we conclude that the kernel of this map is isomorphic to S. In fact, one can show relatively easily that the following sequence is exact:

$$0 \to \mathrm{S} \to D_1 \wedge D_1 \to D_2 \to 0$$

Example 4.6. The smallest non-trivial period polynomial, arising from the cusp form of weight 12, is given by $s_1 2 = X^8Y^2 - 3X^6Y^4 + 3X^4Y^6 - X^2Y^8$. From the short exact sequence, and the isomorphism $\bar{\rho}$, we can immediately see Ihara's relation:

$$3\{\bar{\sigma}_5, \bar{\sigma}_7\} - \{\bar{\sigma}_3, \bar{\sigma}_9\} = 0$$

Using the map $\mathfrak{ls} \to \mathrm{Der}^{\Theta}\mathbb{L}(a, b)$ that sends $\bar{\sigma}_{2n+1}$ to $\epsilon^{\vee}_{2n+2}$, we can apply Pollack's work to describe all such quadratic relations and their connection to modular forms.

Definition 4.7. For f a cusp form of weight n, define the period polynomial of f to be

$$r_f(X, Y) = \sum a_f(k) X^{n-2-k} Y^k = \int_0^{i\infty} f(\tau)(X - \tau Y)^{n-2} d\tau$$

In [32], Zagier extends this definition to all modular forms. Denote by

$$r_f^+ = \frac{1}{2}(r_f(X,Y) + r_f(X,-Y)$$

the even degree part of r_f. This is an element of S. In his thesis, Pollack shows the following, as a special case of his main theorem.

Theorem 4.8. *For n a fixed positive even integer*

$$\sum_{p+q=n+2} \beta(p,q)[\epsilon_p^\vee, \epsilon_q^\vee] = 0$$

if and only if there exists a modular form f of weight n such that

$$r_f^+(X,Y) = \sum p + q = n + 2\beta(p,q)(X^{p-2}Y^{q-2} - X^{q-2}Y^{p-2})$$

This gives us a way of generating relations, in fact all quadratic relations, among the $\bar{\sigma}_{2n+1}$.

Example 4.9. The relation

$$2\{\bar{\sigma}_3, \bar{\sigma}_{13}\} - 7\{\bar{\sigma}_5, \bar{\sigma}_{11}\} + 11\{\bar{\sigma}_7, \bar{\sigma}_9\} = 0$$

arises from the cusp form of weight 16, with even period polynomial

$$2(X^2Y^{12} - X^{12}Y^2) - 7(X^4Y^{10} - X^{10}Y^4) + 11(X^6Y^8 - X^8Y^6)$$

Modular forms and period polynomials also play a role in defining *exceptional generators.* The map

$$\mathbf{e} : \mathrm{S} \to \mathfrak{ls}$$

defines elements $\mathbf{e}_f \in \mathfrak{ls}$ that in some sense describe the failure of relations in $\mathfrak{ls}$ to hold in $\mathfrak{dmr}_0$. For example

$$3\{\sigma_5, \sigma_7\} - \{\sigma_3, \sigma_9\} \in \mathbb{Q}\mathbf{e}_f$$

for f the cusp form of weight 12. Thus, these exceptional elements become vital in computation of the dimension of solution spaces to the double shuffle equations. In fact, we have that the Conjecture 2.38 is equivalent to showing that $\mathbf{e}(S) \subset \mathfrak{dg}$, which was verified by Brown up to weight 20, and that the Lie subalgebra of $\mathfrak{dg}$ generated by the elements $\mathrm{ad}^{2n}(a)(b)$ and $\mathbf{e}_f$ has the homology described in Conjecture 2.38.

4.4 Analytic continuation methods

While not truly featuring in this work, it would be unsatisfactory to discuss the possibility of a rational associator without briefly commenting on some wholly analytic techniques that may be attempted. Single zeta values have, in some sense, an additional "structure", in that they arise as special points of the Riemann ζ-function. But by considering the ζ function at negative integers, we get rational numbers, satisfying the same (known) relations. Thus, $\zeta(-n)$ makes an excellent candidate for the coefficient of $x_1x_0^{n-1}$ in a rational associator Φ. If one could extend multiple zeta values to the negative integers, in such a way as to satisfy both shuffle and stuffle relations, this would define a rational associator. However, current analytic continuations seem to only satisfy stuffle [28], but not shuffle. Thus, we cannot currently exploit this technique.

One possible method we believe to have potential is to invoke Hurwitz multiple zeta functions

$$\zeta(s_1, s_2, \ldots, s_k; a) := \sum_{n_1 > n_2 > \ldots > n_k \geq 0} \frac{1}{n_1^{s_1} n_2^{s_2} \ldots n_{k-1}^{s_{k-1}} (n_k + a)^{s_k}}$$

By considering derivatives with respect to a, one can renormalise a divergent value of the Hurwitz zeta function as a convergent sum of convergent values, and hence continue, analytically, the zeta function to the negative integers.

Example 4.10. We have $\frac{\partial \zeta}{\partial a}(s; a) = -s\zeta(s+1; a)$ and in general

$$\frac{\partial^n \zeta}{\partial a^n}(s; a) = (-1)^n (s)_n \zeta(s+n; a)$$

where $(s)_n := s(s+1)(s+2)(\cdots)(s+n-1)$ is a rising Pochhammer symbol. Thus, upon Taylor expanding $\zeta(s; a)$ around $a = 1$, we get

$$\zeta(s; a) = a^{-s} + \sum_{n=0}^{\infty} \frac{(-a)^n}{n!} (s)_n \zeta(s+n)$$

and hence

$$\zeta(s) = 1 + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} (s)_n \zeta(s+n)$$

allowing us to push convergence into the left half-plane.

To the best of the author's knowledge, this has not been examined thoroughly, bar by [28], and may merit further study.

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