Algebraic features of multiple zeta values

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Abstract

This report aims to present multiple zeta values, a topic which has witnessed a rich mathematical revival and profound breakthroughs in recent years, yet remains cloaked with long-standing conjectures. It is aimed at the undergraduate/first-year postgraduate reader, but we hope that it will be relevant to anyone with curiosity for the subject. The first three chapters introduce the algebraic structure of multiple zeta values in a detailed, rigorous and approachable way. Chapter 4 investigates interpolation (as recently introduced by Yamamoto) and presents a few independent results on the topic. The final chapter gives a glimpse of a more sophisticated approach involving the theory of motives, which has borne powerful results in recent years.

Contents

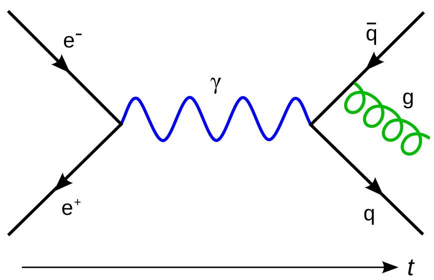
Chapter 1

Introduction

1.1 Motivation

The Riemann zeta function has been a source of much interest since it was introduced by Euler in the 18th century. It plays a central role in analytic number theory, which aims to use analytical (*continuous*) methods to answer questions about numbers (*discrete*). A first and highly compelling example is that of the infinitude of primes, which can be proved using the divergence of Riemann's zeta function at $s = 1$ (c.f. Appendix A.1). From the undergraduate's perspective, this is equally beautiful and entirely different to Euclid's demonstration, offering a profound connection between seemingly distinct areas of mathematics.

The Riemann hypothesis, perhaps the most famous unsolved problem in mathematics, also illustrates the centrality of the zeta function. Less well-known is the function's applications in physics and probability theory. More recently, a generalisation called the *multiple zeta function* was noticed to arise naturally in quantum field theory. The quantum-mechanical interactions of subatomic particles can be pictured using *Feynman diagrams*, an example of which I reproduce from Wikipedia in my own words below.



This diagram represents an electron (e^-) and a positron (e^+) annihilating each other, producing a photon (γ) which becomes a quark-antiquark pair ($q, \bar{q}$), after which the antiquark emits a gluon (g). This is one among many possible interactions of the electron and positron, each of which have a certain probability of taking place. Computing these probability amplitudes "requires the use of rather large and complicated integrals over a large number of variables" (Wikipedia). It turns out that many of these integrals are integer values of the multiple zeta function, which have particularly nice algebraic structure. Many of these can be written in terms of others, so there is a certain redundancy in computing each of them separately. It would be beneficial to develop a rigorous treatment of these values, for numerical approximation is not always sufficient or possible. This requires us to get a better grasp on the relations they satisfy, and perhaps even finding a restricted set of them which generate everything.

It may also benefit physicists in the following way. If one needs to compute not one but thousands of Feynman diagrams (which is very quickly the case once we increase the number of interacting particles), it will be computationally difficult to numerically approximate thousands of seemingly different integrals. But many of them satisfy relations, so expressing all such integrals in terms of a selected few (some sort of *basis*) would cut down enormously the computational power required. We will see in the final chapter that Brown's decomposition algorithm allows us to perform precisely this. As a result, we need to approximate only a few integrals and decompose all others as a rational combination. The caveat is that these rational coefficients may be extremely large and render the computation difficult – although no doubt less so than before.

Finally, the algebraic structure of MZVs is rich yet elusive, cloaked with long-standing conjectures. Studying them has become interesting in its own right. Our aim is to introduce this in a detailed and accessible way, with chapters 4 and 5 serving to go beyond. We have placed many proofs which are long or intuitively obvious in Appendix A, bearing in mind the less experienced. If the reader is familiar with MZVs, they can be skim-read or skipped entirely.

Notation. To begin, a few notational conventions.

- $\mathbb{N} = \{1, 2, 3, \ldots\}$ (not including 0).
- We write 'linear' for $\mathbb{Q}$-linear, instead of the standard $\mathbb{Z}$-linear.
- The numbering of definitions, theorems, remarks etc. is continuous throughout the report. However, equation labelling is used rarely, and as such will be reset at each chapter.
- When we write that "this statement is supported by strong numerical evidence", we mean that it has been checked for MZVs of low weight, usually up to weight 15 or so. More precisely, algorithms that approximate MZVs numerically to high degree (say 10,000 decimal places) validate the statement up to that precision. In particular, we use the computer algebra system PARI/GP originally developed by Henri Cohen and his co-workers at Université Bordeaux I. The *lindep* function in PARI/GP takes any finite number of MZVs and tries to find a linear relation between them with relatively small coefficients. If it fails to do so with high degree precision, it is reasonable to believe that a statement such as "there are no relations between x and y" holds. This is what we mean by the statement being supported by strong numerical evidence.
- All proofs with no further indication are my own. If inspired from somewhere but worked through myself, I will also mention it explicitly.
- Proofs placed in the appendix are referenced in the main body, preceded by the re-stated result. Moreover, a ($\star$) hyperlink to the statement in the body is placed for each proof.

1.2 Multiple Zeta Values

Before defining multiple zeta values, we recall the Riemann zeta function and give an indication as to how they arose historically, before appearing in quantum field theory. For $s \in \mathbb{C}$ (with $Re(s) > 1$ convergence), define $\zeta(s)$ as

$$\zeta(s) = \sum_{n>0} \frac{1}{n^s} \, .$$

The so-called Basel problem, posed in 1644, was to find a closed-form expression for

$$\zeta(2) = \sum_{n>0} \frac{1}{n^2} \, .$$

It went unsolved for almost a century, after which Euler proved that $\zeta(2) = \pi^2/6$ in 1734. Elegant and varied proofs have been found since then, thirty-two (!) of which are nicely presented in [BB]. The result has been extended to all positive *even* integers:

$$\zeta(2n) = \frac{(-1)^{n+1} B_{2n} (2\pi)^{2n}}{2(2n)!}$$

for all $n \in \mathbb{N}$, with B_n a sequence of *rationals* called *Bernoulli numbers*, which we do not need to define for this report. Note that this implies $\zeta(2n) \in \mathbb{Q}[\pi^{2n}]$, i.e. even zeta values are rational multiples of π^{2n}, and in particular are transcendent.

On the other hand, no closed-form expression is known for $\zeta(2n+1)$, $n \in \mathbb{Q}$. Apéry showed in [Apé] that $\zeta(3)$ is irrational, but transcendence remains unknown. For higher values including $\zeta(5)$, even irrationality is out of reach. The overarching conjecture, following [BGF], is the following.

Transcendence conjecture. The numbers

$$\{\pi, \zeta(3), \zeta(5), \ldots\}$$

are algebraically independent, that is, for any integer $k \geq 0$ and any non-zero $f \in \mathbb{Q}[x_0, \ldots, x_k]$ we have

$$f(\pi, \zeta(3), \ldots, \zeta(2k+1)) \neq 0 \, .$$

In particular, the transcendence conjecture implies that odd zeta values are all transcendent. Indeed, take $x_0 = \ldots = x_{k-1} = 0$ (i.e. $f \in \mathbb{Q}[x]$ in one variable). Then we have that $f(\zeta(2k+1)) \neq 0$ for any such polynomial. This is precisely the definition of $\zeta(2k+1)$ being transcendent, and holds for any k!

In an attempt to fathom odd zeta values, Euler used partial fractions extensively to decompose $\zeta(3)$ into a different infinite sum, which we now call the multiple zeta value (MZV) $\zeta(2,1)$, defined as

$$\zeta(2,1) = \sum_{n_1 > n_2 > 0} \frac{1}{n_1^2 n_2^1} \, .$$

The general definition will be given below, but the multiple zeta function can be viewed as a multi-variate generalisation of the Riemann zeta function. We will only consider this function at positive integers, whose values will be called MZVs. Euler discovered that

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

which is not obvious at first sight. In fact, in [Eul] he established a general formula to decompose zeta values into a sum of MZVs, given in the next section. His paper is written in latin, but Harada has recently translated his work into english and modern mathematical languague in [Har].

Definition 1.2.1. A multi-index is a sequence $\mathbf{s} = (s_1, \ldots, s_r) \in \mathbb{Z}^r$. We say the multi-index is positive if $s_i \geq 1$ for all $1 \leq i \leq r$, and admissible if it is positive and $s_1 \geq 2$. Define its weight and length to be

$$wt(\mathbf{s}) = s_1 + \ldots + s_r\,,$$
$$l(\mathbf{s}) = r\,.$$

Definition 1.2.2. A multiple zeta value (MZV) is a real number

$$\zeta(\mathbf{s}) = \sum_{n_1 > \ldots > n_r > 0} \frac{1}{n_1^{s_1} \cdots n_r^{s_r}}$$

associated to an admissible multi-index $\mathbf{s}$. We define the weight and length of $\zeta(\mathbf{s})$ by

$$wt(\zeta(\mathbf{s})) = wt(\mathbf{s})$$
$$l(\zeta(\mathbf{s})) = l(\mathbf{s})\,.$$

We also define $\zeta(\varnothing) = 1$ with $l(1) = wt(1) = 0$ for convenience.

Remark 1.2.3. This is well-defined because the conditions on $\mathbf{s}$ give convergence of the iterated sum, which we leave as an easy exercise for the reader. The proof can be found in [BGF, Lemma 1.13]. Note that for $l(\mathbf{s}) = 1$, the condition is $s_1 \geq 2$, as for the Riemann zeta function.

On the other hand, note that weight and length are *not* well-defined: we have $l(\zeta(2,1)) = 2$, but Euler's result gives us $l(\zeta(2,1)) = l(\zeta(3)) = 1$! We will use this definition for convenience, but must be wary of this caveat.

As indicated by Euler's result, MZVs have relations between them. A few interesting cases are exposed in the section below, but the purpose of this report is not to focus on such 'isolated', mostly combinatorial examples. Later sections will look further into large families of relations including the (extended) double shuffle and Ohno's relations, which are expected to be equivalent and comprise *all* linear relations among MZV's.

1.3 Relations among MZVs

We give two interesting families of relations, namely the sum and cyclic sum formulae. The former relates double (length 2) and single zeta values, while the latter exhibits cyclic structure in general MZVs.

Theorem 1.3.1 (Euler's sum formula)**.** For all $k \geq 3$,

$$\sum_{r=2}^{k-1} \zeta(r, k-r) = \zeta(k)\,.$$

This was proved by Euler in [Eul], with immediate corollary ($k = 3$) being $\zeta(2,1) = \zeta(3)$. The original proof can be found in Harada's translation, but we recommend a more straightforward proof as the case $l = 1$ in [Zud, Theorem 1]. We will not reproduce it here as it is rather uninteresting, involving only 'brute force' partial fraction manipulations. In chapters 2 and 3, we will see that there are more elegant and formal approaches to many such relations. Some of them even have connections to other areas of mathematics including modular forms, which Gangl-Kaneko-Zagier studied in [GKZ].

For k even, there is a further refinement of Euler's formula into even and odd parts, which we detail to give the reader a taste of the methods involved in these more elementary cases. The following theorem was first proved by Nielsen in 1965 [Nie].

Theorem 1.3.2 (Even/odd sum formulae)**.** For $k \geq 4$ even,

$$\sum_{r=2 \text{ even}}^{k-1} \zeta(r, k-r) = \frac{3}{4}\zeta(k)\,,$$
$$\sum_{r=2 \text{ odd}}^{k-1} \zeta(r, k-r) = \frac{1}{4}\zeta(k)\,.$$

A cleaner proof using generating functions and a simple fraction expansion was discovered independently in [GKZ], albeit in a more formal setting. I reproduce the proof, filling in a gap discussed with my supervisor Dr. Gangl. To clarify, it should have been mentioned in the paper that their proof uses Euler's sum formula in the first place, at least in my understanding of it. Otherwise, the reader may be led to believe that their proof gives both the refinement *and* Euler's formula as a corollary, by summing up the two equalities in the theorem. On the contrary, proving the refinement involves *using* Euler's formula.

In any case, I reproduce the proof in the non-formal setting for clarity, filling in many details which they leave for the reader. We first need the following two lemmata.

Lemma 1.3.3. For any $k \geq 4$ and $2 \leq j \leq k-2$ we have

$$\zeta(j, k-j) + \zeta(k-j, j) + \zeta(k) = \sum_{r=2}^{k-1} \left[\binom{r-1}{j-1} + \binom{r-1}{k-j-1} \right] \zeta(r, k-r)\,. \qquad (\dagger)$$

Proof. In Appendix A.1, using a simple partial fraction expansion. □

Definition 1.3.4. Define the generating function of the double zeta values of weight k as

$$T_k(X,Y) = \sum_{r=2}^{k-1} \zeta(r, k-r) X^{r-1} Y^{k-r-1} = \sum_{\substack{r+s=k \\ r \geq 2, s \geq 1}} \zeta(r,s) X^{r-1} Y^{s-1}\,.$$

Lemma 1.3.5. Assuming Euler's sum theorem, we have

$$T_k(X,Y) + T_k(Y,X) + \zeta(k)\frac{X^{k-1} - Y^{k-1}}{X - Y} = T_k(X+Y,Y) + T_k(X+Y,X)$$

for all $k \geq 4$.

Proof. In GKZ it is written that this can easily be concluded from the previous lemma. We give a detailed proof and fill the aforementioned gap in Appendix A.1. □

This lemma immediately implies the even/odd refinement given in theorem 1.3.2, as follows.

Proof. Taking $(X,Y) = (1,0)$ in Lemma 1.3.5 gives us

$$\begin{aligned} T_k(1,0) + T_k(0,1) + \zeta(k) &= T_k(1,0) + T_k(1,1) \\ \zeta(k) &= \sum_{r=2}^{k-1} \zeta(r, k-r)\,, \end{aligned}$$

which is Euler's sum formula. The lemma was proved *using* this formula, so this is a circular conclusion stated only for clarity. We now turn to the refinement theorem. For k even, taking $(X,Y) = (1,-1)$ yields

$$\begin{aligned} \zeta(k) &= -T_k(1,-1) - T_k(-1,1) \\ &= -\sum_{r=2}^{k-1} \zeta(r,k-r)\left[(-1)^{k-r-1} + (-1)^{r-1}\right] \\ &= 2\sum_{r=2}^{k-1} (-1)^r \zeta(r,k-r)\,, \end{aligned}$$

which implies that

$$\frac{1}{2}\zeta(k) = \sum_{r=2 \text{ even}}^{k-1} \zeta(r,k-r) - \sum_{r=2 \text{ odd}}^{k-1} \zeta(r,k-r)\,.$$

Summing and subtracting Euler's formula, we obtain the required equalities:

$$\begin{aligned} \sum_{r=2 \text{ even}}^{k-1} \zeta(r,k-r) &= \frac{3}{4}\zeta(k) \\ \sum_{r=2 \text{ odd}}^{k-1} \zeta(r,k-r) &= \frac{1}{4}\zeta(k)\,. \end{aligned}$$

□

Corollary 1.3.6. For $k = 4$ the sum formula is

$$\zeta(4) = \zeta(3,1) + \zeta(2,2)\,.$$

The refinement theorem moreover gives

$$\zeta(4) = \frac{4}{3}\zeta(2,2) = 4\zeta(3,1)\,,$$

splitting the sum formula into two and reducing both $\zeta(2,2)$ and $\zeta(3,1)$ to a multiple of $\zeta(4)$! This gives a flavour for the fact that despite the large number of MZVs, we can express many of them in terms of a limited set of elements.

Before moving on, we write down a further consequence of lemma 1.3.5 which we discovered.

Proposition 1.3.7. For any $k \geq 3$,

$$\sum_{r=2}^{k-1} (k+1-2^r)\zeta(r, k-r) = 0\,.$$

This implies that any double (length 2) zeta can be expressed as a $\mathbb{Q}$-linear combination of other double zetas through an explicit formula. In particular, for $\zeta(k-1,1)$ we obtain the (new?) expression

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

Proof. We first write

$$\frac{X^{k-1} - Y^{k-1}}{X - Y} = \sum_{j=1}^{k-1} X^{j-1} Y^{k-j-1}\,.$$

Then taking $(X, Y) = (1, 1)$ in lemma 1.3.5 and using Euler's formula, we obtain

$$T_k(1,1) + T_k(1,1) + \zeta(k) \sum_{j=1}^{k-1} 1 \cdot 1 = T_k(2,1) + T_k(2,1)$$

$$2\sum_{r=2}^{k-1} \zeta(r, k-r) + (k-1)\sum_{r=2}^{k-1} \zeta(r, k-r) = 2\sum_{r=2}^{k-1} 2^{r-1}\zeta(r, k-r)$$

$$\sum_{r=2}^{k-1} (k+1-2^r)\zeta(r, k-r) = 0\,.$$

□

Example 1.3.8. Taking $k = 4$, we obtain

$$(5-4)\zeta(2,2) + (5-8)\zeta(3,1) = 0$$
$$\zeta(2,2) = 3\zeta(3,1)\,.$$

Similarly, taking $k = 5$ gives

$$2\zeta(2,3) = 2\zeta(3,1) + 10\zeta(4,1)\,,$$

which is not *a priori* obvious.

Finally, we state two more relations without proof. The first is a generalisation of the sum formula above to arbitrary length. An elementary proof of it can be found in [Gra], but chapter 3 will also reveal it as a special case of Ohno's Theorem. The second is the cyclic sum formula, proved by Hoffman and Ohno in [HO] using partial fractions and "cyclic" derivations. A purely algebraic proof has also been provided by Tanaka-Wakabayashi in [TW].

Theorem 1.3.9 (General sum formula)**.** For all $k \geq 3$,

$$\sum_{\substack{r_1+\ldots+r_n=k \\ r_1\geq 2,\, r_i\geq 1}} \zeta(r_1,\ldots,r_n) = \zeta(k)\,.$$

Note that for $n = 2$, this corresponds to Euler's formula.

Theorem 1.3.10 (Cyclic sum formula)**.** For any positive integers $k_1,\ldots,k_n$ with some $k_i \geq 2$,

$$\sum_{j=1}^{n}\sum_{i=1}^{k_j-1} \zeta(k_j+1-i, k_{j+1},\ldots,k_n,k_1,\ldots,k_{j-1},i) = \sum_{j=1}^{n} \zeta(k_j+1,k_{j+1},\ldots,k_n,k_1,\ldots,k_{j-1})\,.$$

This looks rather complicated but is included to give the reader a taste for the algebraic structure underlying MZV's, and the wealth of relations between them. It has also been shown in [HO] (Corollary 2.4) that the cyclic sum formula implies the sum formula, which is rather astounding at first, given their structural differences.

Remark 1.3.11. In every relation that we have given above, whether in generality or examples, notice that all MZVs which appear have equal weight. For example, the MZVs on the LHS of the general sum formula have weight $r_1+\ldots+r_n = k$, and the RHS is $\zeta(k)$ with the same weight. Although a proof is out of reach for now, numerical experiments suggest that all relations among MZVs are homogeneous in weight, made precise by Conjecture 1.4.4 of the next section.

1.4 The algebra of MZVs

We conclude this chapter by establishing some notation relating to the algebraic structure of MZVs.

Definition 1.4.1. Define $\mathcal{Z}_k = \langle \zeta(\mathbf{s}) \mid wt(\mathbf{s}) = k\rangle_{\mathbb{Q}} := \mathrm{span}_{\mathbb{Q}}\{\zeta(\mathbf{s}) \mid wt(\mathbf{s}) = k\}$, the $\mathbb{Q}$-vector space of MZVs of a fixed weight $k \geq 2$.

For convenience, let $\mathcal{Z}_0 = \mathbb{Q}$ and $\mathcal{Z}_1 = \{0\}$. This agrees with our definition of $\zeta(\varnothing) = 1$, and the fact that no MZVs of weight 1 exist. Indeed $\zeta(1) = \infty$ is not an MZV since (1) is not an admissible multi-index.

Example 1.4.2. The only MZVs of weight 3 are $\zeta(3)$ and $\zeta(2,1)$, so

$$\mathcal{Z}_3 = \{a\zeta(3) + b\zeta(2,1) \mid a,b \in \mathbb{Q}\}\,.$$

Now Euler's identity gives $\zeta(3) = \zeta(2,1)$, so $\mathcal{Z}_3 = \{a\zeta(3) \mid a \in \mathbb{Q}\}$. It follows that $\dim_{\mathbb{Q}}(\mathcal{Z}_3) = 1$!

For another example which further motivates the purpose of finding relations, take $k = 4$. We have four MZV's of this weight: $\zeta(4), \zeta(3,1), \zeta(2,2), \zeta(2,1,1)$. By Corollary 1.3.6, the refinement theorem gives

$$\zeta(4) = 4\zeta(3,1) = \frac{4}{3}\zeta(2,2)\,,$$

so $\mathcal{Z}_4 = \{a\zeta(4) + b\zeta(2,1,1) \mid a,b \in \mathbb{Q}\}$ with $\dim(\mathcal{Z}_4) \leq 2$. With more advanced families of relations from Chapter 2, we will show in Example 2.5.9 that $\dim(\mathcal{Z}_4) = 1$, so we can express all MZVs of weight 4 in terms of $\zeta(4)$!

Definition 1.4.3. Define $\mathcal{Z} = \text{span}_{\mathbb{Q}}\{1, \zeta(2), \zeta(3), \zeta(2,1), \zeta(2,2), \zeta(3,1), \ldots\}$, the vector space of all MZVs (and 1) over $\mathbb{Q}$.

Extensive numerical experiments suggest that no linear relations exist between MZVs of different weight, and moreover that all MZVs are irrational. This would imply $\mathcal{Z}_n \cap \mathcal{Z}_m = \{0\}$ for all $n \neq m$, which can be written as follows.

Conjecture 1.4.4. We have a direct sum decomposition $\mathcal{Z} = \bigoplus_{k \geq 0} \mathcal{Z}_k$.

In the next section it will be established that $\mathcal{Z}$ is an algebra, namely that there exists a bilinear product $* : \mathcal{Z} \times \mathcal{Z} \to \mathcal{Z}$. In fact, the product will respect the weight in the sense that $* : \mathcal{Z}_n \times \mathcal{Z}_m \to \mathcal{Z}_{n+m}$ for all $n, m \geq 0$. We can also write this as $\mathcal{Z}_n * \mathcal{Z}_m \subseteq \mathcal{Z}_{n+m}$, which turns $\mathcal{Z}$ into a *graded* algebra. In particular, we obtain the following result.

Proposition 1.4.5. Conjecture 1.4.4 implies that all multiple zeta values are transcendent.

Proof. (Following [BGF, Remark 1.42]) Assume $\zeta(\mathbf{s}) \in \mathcal{Z}_k$ is algebraic, for some $\mathbf{s}$ of weight $k > 0$. By definition, there exist $a_0, \ldots, a_n \in \mathbb{Q}$ with $a_n \neq 0$ such that $\sum_{i=0}^{n} a_i \zeta(\mathbf{s})^i = 0$. Rearranging gives $a_n \zeta(\mathbf{s})^n = -\sum_{i=0}^{n-1} a_i \zeta(\mathbf{s})^i$, and by the grading above we have the LHS in $\mathcal{Z}_{nk}$ and the RHS in $\bigoplus_{i=0}^{n-1} \mathcal{Z}_{ik}$. If the conjecture 1.4.4 holds, these vector spaces have empty intersection, so $a_n \zeta(\mathbf{s})^n \in \mathcal{Z}_{nk} \cap \bigoplus_{i=0}^{n-1} \mathcal{Z}_{ik} = \{0\}$. Finally $a_n \zeta(\mathbf{s})^n = 0$ implies $a_n = 0$, a contradiction. □

Above, we have seen that the relation $\zeta(2,1) = \zeta(3)$ implies $\dim_{\mathbb{Q}}(\mathcal{Z}_3) = 1$. What is the dimension for general $\mathcal{Z}_k$? A priori, the dimension may grow very quickly with k, since the number of MZVs grows exponentially with weight, as made explicit by the following proposition.

Proposition 1.4.6. For $k \geq 2$, the number of admissible multi-indices of weight k is 2^{k-2}.

Proof. There is a more elegant proof relying on the binary sequence associated to a multi-index, but we will only introduce these in chapter 2. The proof of Corollary 3.1.6 will resemble this more elegant method, but we give an elementary argument in Appendix A.1. □

In other words, this proposition states that we would have $\dim_{\mathbb{Q}}(\mathcal{Z}_k) = 2^{k-2}$ if there were no relations between MZVs at all. This is not the case, and finding a new relation may reduce the dimension by 1 by expressing one MZV in terms of others, as in the case of $\mathcal{Z}_3$.

The family of relations we shall obtain in the next chapter will also increase rapidly with k, slowing down the growth of dimension considerably. This can help us give an upper bound on dimension, but lower bounds would require proving that certain MZVs are linearly independent over $\mathbb{Q}$, which is currently out of reach. We give the conjectured dimension of $\mathcal{Z}_k$, which has recently been proved to be an upper bound.

Definition 1.4.7. The Fibonacci-like sequence $(d_k)_{k\geq 0}$ is defined recursively by $d_0 = d_2 = 1$, $d_1 = 0$ and

$$d_k = d_{k-2} + d_{k-3}$$

for all $k \geq 3$.

The following conjecture is supported by overwhelming numerical evidence, first formulated by Zagier in [Zag, p. 493] "after many discussions with Drinfel'd, Kontsevich and Goncharov".

Zagier's Conjecture. For all $k \geq 0$,

$$\dim_{\mathbb{Q}}(\mathcal{Z}_k) = d_k \,.$$

The following table gives the first few values of d_k, as well as 2^{k-2} for comparison.

k	2	3	4	5	6	7	8	9	10	11	12	13	14
d_k	1	1	1	2	2	3	4	5	7	9	12	16	21
2^{k-2}	1	2	4	8	16	32	64	128	256	512	1024	2048	4096

Table 1.1: Small values of d_k.

The following impressive result was discovered independently by Terasoma [Ter] and Deligne-Goncharov [DG]. Proving it involves the sophisticated theory of motives, discussed shortly in Chapter 5.

Theorem 1.4.8. For all $k \geq 0$,

$$\dim_{\mathbb{Q}}(\mathcal{Z}_k) \leq d_k \,.$$

This is very encouraging. On the other hand, a lower bound seems completely out of reach: it has not been proved that $\dim_{\mathbb{Q}}(\mathcal{Z}_k) > 1$ for any single $k \geq 2$, despite the overwhelming numerical evidence that d_k is the lower bound!

Beyond dimension, one can ask about whether we can find a basis for $\mathcal{Z}_k$. Define *Hoffman's family* to be

$$B = \{\zeta(s_1, \ldots, s_r) \mid s_i \in \{2, 3\}$$

and

$$B_k = \{\zeta(s_1, \ldots, s_r) \mid s_i \in \{2, 3\},\, wt(s_1, \ldots, s_r) = k\} = B \cap \mathcal{Z}_k$$

for $k \geq 2$, with $B_0 := \{1\}$ and $B_1 := \{0\}$. Hoffman gave the following refinement of Zagier's conjecture in [Hof2, Conj. C].

Hoffman's Conjecture. B_k is a $\mathbb{Q}$-basis for $\mathcal{Z}_k$.

This conjecture is based on the fact that the number of elements in B_k is d_k, as the following counting exercise demonstrates.

Proposition 1.4.9. For any $k \geq 2$, $|B_k| = d_k$.

Proof. First note that $|B_0| = |B_2| = 1 = d_2 = d_0$ and $|B_1| = 0 = d_1$. For $k \geq 3$, the number of admissible multi-indices with $2, 3$ as entries corresponds to the number of solutions to the equation

$$k = a_1 + \ldots + a_n$$

with $n \geq 1$ and $a_i \in \{2, 3\}$. Once we choose a_1 to be 2 or 3, we have

$$k - a_1 = a_2 + \ldots + a_n$$

which has $|B_{k-a_1}|$ solutions. Summing over both choices,

$$|B_k| = |B_{k-2}| + |B_{k-3}| = d_{k_2} + d_{k-3} = d_k \,. \qquad \square$$

Hoffman's conjecture is widely believed to hold, supported by strong numerical evidence. Proving linear independence of certain MZVs is beyond our grasp (as for lower bounds), and so this conjecture stands. Nevertheless, a major breakthrough was achieved recently by Brown in [Bro1], proving the 'spanning' half of this conjecture.

Brown's Theorem. Any MZV can be written as a $\mathbb{Q}$-linear combination of $\zeta(s_1, \ldots, s_r)$ with $s_i \in \{2, 3\}$ for all i. In other words,

$$\text{span}_{\mathbb{Q}}\{B_k\} = \mathcal{Z} \,.$$

It now follows that Theorem 1.4.8 is in fact a corollary to Brown's Theorem, since the number of elements in B_k is d_k. Moreover, a spanning set of d_k elements in a vector space of dimension d_k must be a basis by elementary linear algebra, so Hoffman's family will form a basis for $\mathcal{Z}_k$ if Zagier's conjecture holds.

One should notice the parallel between Theorem 1.4.8 being half of Zagier's conjecture, and Brown's Theorem being half of Hoffman's conjecture. Nonetheless, Brown's theorem is much stronger and gives explicit elements which we can manipulate, not least with the foreshadowed applications in physics.

Chapter 2

Shuffle and stuffle products

In this chapter we introduce the *shuffle* and *stuffle* products. Each of these is a way of expressing the product of two MZVs as a linear combination of other MZVs. As foreshadowed in the previous chapter, this turns $\mathcal{Z}$ into a graded algebra. Moreover, comparing the two products will produce a powerful family named *double shuffle* relations. The first three sections are almost entirely devoid of explicit references, but the content was developed mostly by Hoffman. We follow [Hof2] for definitions and the like, but re-write everything in our own words.

2.1 Sum representation and stuffle

We begin with a simple illustration of the stuffle product with MZVs of length 1. For integers $a, b > 1$, we have

$$\zeta(a)\zeta(b) = \sum_{n>0} \frac{1}{n^a} \sum_{m>0} \frac{1}{m^b} = \sum_{\substack{n>0\\m>0}} \frac{1}{n^a m^b} \ .$$

Splitting this sum according to the cases $n > m$, $n < m$ and $n = m$ gives us

$$\begin{aligned}\zeta(a)\zeta(b) &= \sum_{n>m>0} \frac{1}{n^a m^b} + \sum_{m>n>0} \frac{1}{n^a m^b} + \sum_{n=m>0} \frac{1}{n^{a+b}} \\ &= \zeta(a, b) + \zeta(b, a) + \zeta(a + b) \, .\end{aligned}$$

Such a splitting holds for general multi-indices $\mathbf{a} = (a_1, \ldots, a_r), \mathbf{b} = (b_1, \ldots, b_s)$. We have

$$\zeta(\mathbf{a})\zeta(\mathbf{b}) = \sum_{\substack{n_1>\ldots>n_r>0\\m_1>\ldots>m_s>0}} \frac{1}{n_1^{a_1} \cdots n_r^{a_r} \cdot m_1^{b_1} \cdots m_s^{b_s}} \ .$$

As with the previous splitting of n and m, this sum does not distinguish between the cases $n_i > m_j$, $n_i < m_j$ and $n_i = m_j$ for each pair (n_i, m_j). Indeed, the sum imposes an ordering between the n_i and an ordering between the m_j, but not in between each other. Each choice will produce an MZV. For instance, $n_1 = m_1 > \ldots > m_s > n_2 > \ldots > n_r$ gives us

$$\sum_{n_1=m_1>\ldots>m_s>n_2>\ldots>n_r>0} \frac{1}{n_1^{a_1+b_1} m_1^{b_1} \cdots m_s^{b_s} n_2^{a_2} \cdots n_r^{a_r}} = \zeta(a_1 + b_1, b_2, \ldots, b_s, a_2, \ldots, a_r) \, .$$

Summing over all possible choices for pairs (i,j), each of which produces an MZV, the product $\zeta(\mathbf{a})\zeta(\mathbf{b})$ will expand into a linear combination. [Think *shuffling* two sets of cards with *st*icking ("$=$") allowed]. As a result, $\zeta(\mathbf{a})\zeta(\mathbf{b}) \in \mathcal{Z}$ or equivalently, $\mathcal{Z} \cdot \mathcal{Z} \subseteq \mathcal{Z}$. This turns $\mathcal{Z}$ into an algebra, as previously indicated.

Remark 2.1.1. We cannot choose orderings between pairs (n_i, m_j) arbitrarily, since the orderings $n_1 > \ldots > n_r$ and $m_1 > \ldots > m_s$ must be respected. For instance we cannot choose $n_1 < m_1$ and $m_1 < n_2$, since then $n_1 < n_2$ violates the initial order.

We would like to make the set of admissible orderings rigorous, so as to write the product more explicitly. A first step is to notice the inductive structure of the pairing process, performed on $n = l(\mathbf{a}) + l(\mathbf{b}) = r + s$ as follows. (†)

First make a pairing choice between n_1 and m_1, which gives us three cases $n_1 > m_1$, $n_1 < m_1$ or $n_1 = m_1$. In the first case, all pairings of the type (n_1, m_j) are determined (no freedom), since $n_1 > m_1 > m_j$ for all $j \geq 1$. Therefore n_1 is 'eliminated' and it remains only to choose orderings between $(n_2, \ldots, n_r)$ and $(m_1, \ldots, m_s)$, which reduces n to $n-1 = (r-1)+s$. The second and third cases give similar reduction to $n-1 = r+(s-1)$ and $n-2 = (r-1)+(s-1)$ respectively. To make this process formal, we introduce the 'harmonic' algebra.

2.2 The harmonic algebra

The first two definitions are inspired from [BGF, Sec. 1.6].

Definition 2.2.1. Let $A = \{a_i \mid i \in I\}$ a set. If I is countable, we call A an *alphabet* and a_i its *letters*. For any such alphabet, define the free monoid A^* whose elements are all finite *words* from A (strings of letters), with concatenation as its binary operation. More precisely,

$$A^* = \{a_{i_1} \ldots a_{i_r} \mid r \geq 0,\ a_{i_k} \in A\}$$

with identity the empty word 1 ($r = 0$) and concatenation product:

$$a_{i_1} \ldots a_{i_r} \cdot b_{j_1} \ldots b_{j_s} = a_{i_1} \ldots a_{i_r} b_{j_1} \ldots b_{j_s} \qquad \forall\, a_{i_k}, b_{j_k} \in A\,.$$

Definition 2.2.2. Given an alphabet A, write $\mathbb{Q}\langle A \rangle$ the $\mathbb{Q}$-vector space generated by A^*, i.e. whose basis elements are words in the alphabet A. More precisely,

$$\mathbb{Q}\langle A \rangle = \{q_1 w_1 + \ldots + q_n w_n \mid n \geq 0, q_i \in \mathbb{Q}, w_i \in A^*\}\,.$$

This forms an algebra (a vector space equipped with a bilinear operation) once endowed with the concatenation product above, extended linearly. Extending our linguistic terminology, we call *sentences* the elements $w \in \mathbb{Q}\langle A \rangle$, with w a word if and only if $w \in A^*$.

We define the *harmonic algebra* as in [Hof2, Chap. 2].

Definition 2.2.3. Taking $A = \{x, y\}$ above, the harmonic algebra is defined as $\mathfrak{h} := \mathbb{Q}\langle x, y\rangle$. Moreover, let $\mathfrak{h}^1 := \mathfrak{h}y$ the algebra generated by *positive* words (those ending in y), and $\mathfrak{h}^0 := x\mathfrak{h}^1 = x\mathfrak{h}y$ the algebra generated by *admissible* words (those ending in y and beginning in x).

Finally, define the *weight* of a word to be $wt(a_{i_1} \ldots a_{i_r}) = r$. It would seem more natural to call this the *length* of a word, but we will see the usefulness of this terminology later.

Remark 2.2.4. We leave it as an easy exercise to check that $\mathfrak{h}$ is indeed an algebra with identity 1, and that $\mathfrak{h}^0 \subset \mathfrak{h}^1 \subset \mathfrak{h}$ are sub-algebras.

The connection between MZVs and this algebraic setting will soon be made clear. This final definition will make the relationship more explicit and intuitive.

Definition 2.2.5. Let $z_n = x^{n-1}y := \underbrace{x \ldots x}_{n-1} y$ and $\mathcal{A} = \{z_n \mid n \in \mathbb{N}\}$.

The reader should think of words in $\mathcal{A}^*$ as corresponding to multi-indices through the following bijection:

$$z_{s_1} \ldots z_{s_r} \leftrightarrow (s_1, \ldots, s_n)\,.$$

The proposition below allows us to extend this correspondence to $\mathfrak{h}^1$.

Proposition 2.2.6. Any word $w \in \mathfrak{h}^1$ can be written as $w = z_{i_1} \ldots z_{i_m}$ with $i_1, \ldots, i_m \in \mathbb{N}$. This turns $\mathcal{A}$ into a generating set for $\mathfrak{h}^1$, i.e. $\mathfrak{h}^1 = \mathbb{Q}\langle \mathcal{A}\rangle$.

Proof. By induction on $k := \#\{\text{number of } y\text{'s in } w\}$. For $k = 0$ we must have $w = 1$ since $\mathfrak{h}^1 = \mathfrak{h}y$, so we are done by taking $m = 0$ in the proposition. For the induction step, take any word w with $\#y = k + 1 \geq 1$. Since $w \in \mathfrak{h}y$, write $w = w'y$ with $w' \in \mathfrak{h}$. Let $i \geq 0$ the number of x's at the end of w' before we either reach a y or the word finishes. Then $w' = w''z_{i+1}$ with $w'' \in \mathfrak{h}^1$, which concludes the induction since w'' has $\#y = k$. □

Definition 2.2.7. Define the *length* of a word $w = z_{i_1} \ldots z_{i_m} \in \mathfrak{h}^1$ to be $l(w) = m$ (or equivalently, its number of letters y). Note that $wt(w) = i_1 + \ldots + i_m$, mirroring the definitions of weight and length for multi-indices.

We can now think of words in $\mathfrak{h}^1$ as multi-indices, and words in $\mathfrak{h}^0 \subseteq \mathfrak{h}^1$ as admissible multi-indices. Indeed, words $w \in \mathfrak{h}^0$ begin with an x, so that $w = z_{s_1} \ldots z_{s_m}$ with $s_1 \geq 2$. This corresponds bijectively to the multi-index $(s_1, \ldots, s_m)$, which is admissible since $s_1 \geq 2$! This makes explicit the relationship between the harmonic algebra and MZVs. The *raison d'être* of this formalism is that letters, words and sentences are more convenient to work with than indices, multi-indices and their 'sum' respectively. For instance, indices are separated by commas and enclosed by parentheses, whereas the former are simply concatenated.

Note that we have defined a correspondence between admissible multi-indices and words in $\mathfrak{h}^0$, but need a way to 'plug' these into the ζ function. The following map plays precisely this role.

Definition 2.2.8. Define the map $Z^* : \mathfrak{h}^0 \longrightarrow \mathbb{R}$ such that $Z^*(z_{s_1} \ldots z_{s_n}) = \zeta(s_1, \ldots, s_n)$ and $Z^*(1) = 1$, extended linearly to sentences.

With this formalised correspondence in hand, any operation we define on $\mathfrak{h}^1$ can be defined only through words in $\mathcal{A}^*$, which correspond to MZVs. The following definition will help us settle the initial goal of finding a way to express the product of MZVs formally, mimicking the inductive pairing process described in (†).

First define the (commutative) circle product $\circ$ on $\mathcal{A}$ as $z_n \circ z_m = z_{n+m}$.

Definition 2.2.9. The stuffle product $*$ on $\mathfrak{h}^1$ is defined recursively by:

$$\begin{aligned} 1 * u = u * 1 &= u \\ z_n u * z_m v &= z_n(u * z_m v) + z_m(z_n u * v) + (z_n \circ z_m)(u * v) \end{aligned}$$

for all words $u, v \in \mathfrak{h}^1$, extended linearly to all sentences, and with concatenation $\cdot$ left implicit by juxtaposition of terms.

Remark 2.2.10. One must check that this is well-defined, i.e. that $w * w' \in \mathfrak{h}^1$ (not $\mathfrak{h}$!) for all $w, w' \in \mathfrak{h}^1$. This can easily be done by induction on the sum of word lengths.

Proposition 2.2.11. The stuffle product is associative and commutative, turning $(\mathfrak{h}^1, *)$ into a commutative algebra with product $*$. Moreover, $\mathfrak{h}^0$ is a sub-algebra of $\mathfrak{h}^1$ with respect to $*$.

Proof. These claims can easily be proved by induction. See [Hof2, Theorem 2.1] for details. □

Example 2.2.12. We give a simple example of the stuffle product. Let $a = xyy, b = xy \in \mathfrak{h}^1$. First write a and b in the basis $\mathcal{A}$, giving $a = z_2 z_1, b = z_2$. Then we obtain:

$$\begin{aligned} a * b &= z_2(z_1 * z_2) + z_2(z_2 z_1 * 1) + z_{2+2}(z_1 * 1) \\ &= z_2\left[z_1(1 * z_2) + z_2(z_1 * 1) + z_{1+2}(1 * 1)\right] + z_2 z_2 z_1 + z_4 z_1 \\ &= z_2 z_1 z_2 + 2 z_2 z_2 z_1 + z_2 z_3 + z_4 z_1 \,. \end{aligned}$$

Example 2.2.13. For $a, b \geq 1$,

$$z_a * z_b = z_a(1 * z_b) + z_b(z_a * 1) + z_{a+b}(1 * 1) = z_a z_b + z_b z_a + z_{a+b} \,.$$

But by our correspondence, we can view this equation (for $a, b \geq 2$) as representing

$$\zeta(a * b) = \zeta(a, b) + \zeta(b, a) + \zeta(a + b) \,,$$

so that replacing $\zeta(a * b)$ by $\zeta(a)\zeta(b)$ would give us

$$\zeta(a)\zeta(b) = \zeta(a, b) + \zeta(b, a) + \zeta(a + b) \,,$$

which is true by the very first example of MZV products in this chapter.

The example above suggests that this mysterious 'stuffle' product imitates the behaviour of MZV products. This holds in full generality, made precise by the following theorem.

Theorem 2.2.14 (Following [Hof2])**.** The map $Z^* : (\mathfrak{h}^0, *) \longrightarrow (\mathbb{R}, \cdot)$ is a $\mathbb{Q}$-algebra homomorphism.

It is sometimes useful to write Z^* as ζ, so that $\zeta(z_{s_1}\dots z_{s_n}) \coloneqq \zeta(s_1,\dots,s_n)$.

Remark 2.2.15. The map Z^* is well-defined: $z_{s_1}\dots z_{s_n} \in \mathfrak{h}^0 \implies z_{s_1}$ starts with an $x \implies s_1 \geq 2 \implies \zeta(s_1,\dots,s_n)$ converges.

For the proof, it will be useful to define the 'truncated' MZVs as follows.

Definition 2.2.16. For an admissible multi-index $\mathbf{a} = (a_1,\dots,a_r)$, define the corresponding 'p-truncated' MZV as

$$\zeta_p(\mathbf{a}) = \sum_{p>n_1>\ldots>n_r>0} \frac{1}{n_1^{a_1}\cdots n_r^{a_r}}$$

and the corresponding map $Z_p^* : (\mathfrak{h}^0, *) \longrightarrow (\mathbb{R}, \cdot)$ such that $Z_p^*(z_{a_1}\dots z_{a_r}) = \zeta_p(a_1,\dots,a_r)$.

Remark 2.2.17. We have $\lim_{p\to\infty} \zeta_p(\mathbf{a}) = \zeta(\mathbf{a})$. Thus for any word $w_i = z_{a_1}\dots z_{a_r} \in \mathfrak{h}^0$,

$$\lim_{p\to\infty} Z_p^*(w_i) = \lim_{p\to\infty} \zeta_p(a_1,\dots,a_r) = \zeta(a_1,\dots,a_r) = Z^*(w_i)\,.$$

Moreover, any element $w \in \mathfrak{h}^0$ is as a linear combination of words w_i and we obtain

$$\begin{aligned}\lim_{p\to\infty} Z_p^*(w) = \lim_{p\to\infty} Z_p^*\left(\sum_{i=1}^n c_i w_i\right) &= \sum_{i=1}^n c_i \lim_{p\to\infty} Z_p^*(w_i) \\ &= \sum_{i=1}^n c_i Z^*(w_i) = Z^*\left(\sum_{i=1}^n c_i w_i\right) = Z^*(w)\,.\end{aligned}$$

Proof of Theorem. In Appendix A.2, proving a necessary lemma along the way. □

The proof looks elaborate, but is really a technical way of representing a simple inductive process: to take the product of two MZVs, pull out the leftmost index of each to obtain three terms, and repeat until we reach the end. The following example illustrates the power of our theorem.

Example 2.2.18. We want to decompose $\zeta(2,1)\zeta(2)$ into a linear combination of MZVs. By example 2.2.12, we have

$$z_2z_1 * z_2 = z_2z_1z_2 + 2z_2z_2z_1 + z_4z_1\,.$$

Now using Theorem 2.2.14,

$$\begin{aligned}Z^*(z_2z_1 * z_2) &= Z^*(z_2z_1z_2 + 2z_2z_2z_1 + z_2z_3 + z_4z_1) \\ Z^*(z_2z_1)Z^*(z_2) &= Z^*(z_2z_1z_2) + 2Z^*(z_2z_2z_1) + Z^*(z_2z_3)Z^*(z_4z_1) \\ \zeta(2,1)\zeta(2) &= \zeta(2,1,2) + 2\zeta(2,2,1) + \zeta(2,3) + \zeta(4,1)\,,\end{aligned}$$

which linearises the product as required!

Corollary 2.2.19. $(\mathcal{Z},\cdot)$ is a graded algebra.

Technically speaking, a graded algebra should also have direct sum decomposition, which is the content of conjecture 1.4.4, but we abuse the name for convenience. I supply this corollary with my own proof in Appendix A.2.

2.3 Integral representation and shuffle

The previous section establishes that $\mathcal{Z}$ is a graded algebra, a testimony to the rich algebraic structure of MZVs. However, the stuffle product only gave us information about how to decompose the product of MZVs. It does not provide any linear relations between them (say $\zeta(3) = \zeta(2,1)$, unlike the sum or cyclic sum theorems. Finding a second way to express products, however, would produce a linear relation by equating the two distinct decompositions.

The aim of the following two sections is precisely to construct a second product, namely the *shuffle*. This relies on representing MZVs as integrals, rather than sums. Comparing stuffle and shuffle will produce a large family of relations between MZV's called *double shuffle* relations. We must first introduce the integral formulation of MZVs, with a motivating example as follows.

Example 2.3.1. We illustrate the integral representation of $\zeta(2)$ by considering the expression

$$\int\limits_{1>t_1>t_2>0} \frac{dt_1}{t_1}\,\frac{dt_2}{1-t_2}\,.$$

Expanding in power series and integrating twice gives

$$\begin{aligned}\int\limits_{1>t_1>t_2>0} \frac{dt_1}{t_1}\,\frac{dt_2}{1-t_2} &= \int\limits_0^1 \frac{dt_1}{t_1}\int\limits_0^{t_1}\sum_{n\geq 0} t_2^n dt_2 = \sum_{n\geq 0}\int\limits_0^1 \frac{dt_1}{t_1}\left[\frac{t_2^{n+1}}{n+1}\right]_0^{t_1} \\ &= \sum_{n\geq 0}\int\limits_0^1 \frac{t_1^n}{n+1}dt_1 = \sum_{n\geq 0}\frac{1}{(n+1)^2} = \zeta(2)\,,\end{aligned}$$

which realises $\zeta(2)$ as an integral.

This can be done in full generality. First, we associate to any admissible multi-index $\mathbf{a}$ the 'binary' sequence $\bar{\mathbf{a}}$:

$$(a_1,\ldots,a_r) = \mathbf{a} \;\leftrightarrow\; \bar{\mathbf{a}} = x^{a_1-1}y\ldots x^{a_r-1}y \in \mathfrak{h}^0$$

This is just our usual correspondence between multi-indices and words in $\mathfrak{h}^0$: $\bar{\mathbf{a}} = z_{a_1}\ldots z_{a_r}$. Nonetheless, it is crucial to the integral formulation that we use x and y explicitly instead of z. Also note that the number of letters x, y in $\bar{\mathbf{a}}$ is equal to $a_1 + \ldots + a_r = wt(\mathbf{a})$, so defining the length as such gives $l(\bar{\mathbf{a}}) = wt(\mathbf{a})$.

We define the differential forms

$$\omega_x(t) = \frac{dt}{t} \qquad \text{and} \qquad \omega_y(t) = \frac{dt}{1-t}\,.$$

Think of them as expressions of the form $f(t_1,\ldots,t_n)dt_1\ldots dt_n$ with f continuous, which we can integrate over a domain. In other words, view differential forms as arguments for the integral operator over a given domain. For example, taking $\omega(t) = t^2 dt$ with domain $[0,1] \subset \mathbb{R}$ gives

$$\int_0^1 (\omega) = \left[\frac{t^3}{3}\right]_0^1 = \frac{1}{3}\,.$$

If the reader is familiar with these: strictly speaking, we won't be working with differential forms and their wedge product. Instead we use the term 'differential form' as a convenient shorthand for a function times an infinitesimal quantity, of which we can take the Lebesgue integral.

For any admissible multi-index $\mathbf{s}$ with weight n, write its binary sequence as $\bar{\mathbf{s}} = \epsilon_1 \dots \epsilon_n$ with $\epsilon_i \in \{x, y\}$, and consider the iterated integral

$$I(\mathbf{s}) := \int_{\Delta^n} \omega_{\epsilon_1}(t_1) \cdots \omega_{\epsilon_n}(t_n) = \int\limits_{1>t_1>\ldots>t_n>0} \omega_{\epsilon_1}(t_1) \cdots \omega_{\epsilon_n}(t_n) \ ,$$

where $\Delta^n = \{(t_1, \dots, t_n) \in \mathbb{R}^n \mid 1 > t_1 > \ldots > t_n > 0\}$ is the standard open n-simplex. The following theorem establishes that MZVs can be written as iterated integrals.

Theorem 2.3.2 (Kontsevich)**.** $I(\mathbf{s}) = \zeta(\mathbf{s})$ for any admissible $\mathbf{s}$.

The proof is not hard, involving simply an inductive generalisation of Example 2.3.1 above. Although Kontsevich's insight is central to the entire study of MZVs, there is no more to the proof than the power series expansion of $(1-t)^{-1}$. We refer to [Hen, App. B.1] for details.

As for the sum formulation, we turn to considering the product of two MZVs $\zeta(\mathbf{a})\zeta(\mathbf{b})$. Writing $\bar{\mathbf{a}} = \alpha_1 \dots \alpha_n$ and $\bar{\mathbf{b}} = \beta_1 \dots \beta_m$, we obtain

$$\begin{aligned}\zeta(\mathbf{a})\zeta(\mathbf{b}) &= \int_{\Delta^{wt(\mathbf{a})}} \omega_{\alpha_1}(t_1) \cdots \omega_{\alpha_n}(t_n) \int_{\Delta^{wt(\mathbf{b})}} \omega_{\beta_1}(t_1) \cdots \omega_{\beta_m}(t_m) \\ &= \int\limits_{\substack{1>t_1>\ldots>t_n>0 \\ 1>t_{n+1}>\ldots>t_{n+m}>0}} \omega_{\alpha_1}(t_1) \cdots \omega_{\alpha_n}(t_n)\, \omega_{\beta_1}(t_{n+1}) \cdots \omega_{\beta_m}(t_{n+m}) \,,\end{aligned}$$

where we have rewritten $t_j = t_{n+j}$ for the second integral. As in the first section with the product of sums, this can be split according to orderings between t_i's and t_j's for $1 \le i \le n$ and $n+1 \le j \le n+m$. Each valid choice will give us an integral over a single simplex, which will again reduce to an MZV by Kontsevich's formula, so that the product can be written as a linear combination. For the integral formulation, this is much easier to make rigorous.

Definition 2.3.3. The shuffle permutation set of $(n, m) \in \mathbb{N} \times \mathbb{N}$ is defined as

$$Sh(n,m) = \left\{ \sigma \in S_{n+m} \;\middle|\; \begin{matrix} \sigma(1) < \ldots < \sigma(n) \\ \sigma(n+1) < \ldots < \sigma(n+m) \end{matrix} \right\} .$$

We view these permutations as acting on binary sequences (in x, y) of length $n+m$ in the following way:

$$\sigma(\epsilon_{i_1} \dots \epsilon_{i_{n+m}}) = \epsilon_{\sigma(i_1)} \dots \epsilon_{\sigma(i_{n+m})}$$

for $i_k \in \{1, \dots, n+m\}$ and $\epsilon_{i_k} \in \{x, y\}$. Note that there are $n+m$ differential forms in the product $\zeta(\mathbf{a})\zeta(\mathbf{b})$ above, and so we view these shuffle permutations as a choice of orderings between t_i, each t_i accompanying a differential form. In the MZVs, this corresponds to ordering the binary sequences $\bar{\mathbf{a}}$ and $\bar{\mathbf{b}}$, which when concatenated have length $l(\bar{\mathbf{a}}) + l(\bar{\mathbf{b}}) = wt(\mathbf{a}) + wt(\mathbf{b}) = n+m$. In this light, we state the following proposition.

Proposition 2.3.4. For any admissible multi-indices $\mathbf{a}, \mathbf{b}$ of weights n, m respectively,

$$\zeta(\mathbf{a})\zeta(\mathbf{b}) = \sum_{\sigma \in \mathrm{Sh}(n,m)} \zeta\left(\sigma^{-1}\left(\bar{\mathbf{a}}\bar{\mathbf{b}}\right)\right) .$$

Remark 2.3.5. We use the notation $\zeta(\bar{\mathbf{a}}) \coloneqq \zeta(\mathbf{a})$ as before, noting that $\bar{\mathbf{a}} \in \mathfrak{h}^0$. One must check that the expression above is well-defined, namely that $\sigma^{-1}\left(\bar{\mathbf{a}}\bar{\mathbf{b}}\right) \in \mathfrak{h}^0$ for all $\sigma \in \mathrm{Sh}(n,m)$ (otherwise some zeta value will not converge). I give a proof as follows.

Since $\mathbf{a}, \mathbf{b}$ are admissible, $\bar{\mathbf{a}}$ and $\bar{\mathbf{b}}$ must begin with an x, therefore $\epsilon_1 = \epsilon_{n+1} = x$. Now the first letter of $\sigma^{-1}(\bar{\mathbf{a}}\bar{\mathbf{b}})$ is $\epsilon_{\sigma^{-1}(1)}$. Using the property $\sigma(1) < \ldots < \sigma(n)$ and $\sigma(n+1) < \ldots < \sigma(n+m)$, we must have $\sigma(1) = 1$ or $\sigma(n+1) = 1$, i.e. $\sigma^{-1}(1) \in \{1, n+1\}$. Thus $\epsilon_{\sigma^{-1}(1)} = x$, which implies that $\sigma(\bar{\mathbf{a}}\bar{\mathbf{b}})$ begins with an x, and finally $\zeta(\sigma(\bar{\mathbf{a}}\bar{\mathbf{b}}))$ converges.

Proof of Proposition. In Appendix A.2. □

As before, we make this formal through the harmonic algebra, following [Hof2]. This is both more elegant than the above, and useful in order to compare it to the stuffle product.

Definition 2.3.6. The shuffle product ш on $\mathfrak{h}$ is defined recursively by:

$$\begin{aligned} 1 \,ш\, w = w \,ш\, 1 = w * 1 \\ aw \,ш\, bw' = a(w \,ш\, bw') + b(aw \,ш\, w') \end{aligned}$$

for all words $w, w' \in \mathfrak{h}$ and $a, b \in \{x, y\}$.

Proposition 2.3.7. The shuffle product is associative and commutative. Moreover, $\mathfrak{h}^0$ is a sub-algebra of $\mathfrak{h}^1$ with respect to ш.

Remark 2.3.8. We can now appreciate the usefulness of having defined $\mathfrak{h}$ through $A = \{x, y\}$ rather than $\mathcal{A} = \{z_n \mid n \in \mathbb{N}\}$, since the shuffle product is defined through its *binary* form instead of z_n's.

Example 2.3.9. We give a simple example of the shuffle product. Let $a = xyy, b = xy \in \mathfrak{h}^1$, as in example 2.2.12. Then

$$\begin{aligned} a \,ш\, b &= x(yy \,ш\, xy) + x(xyy \,ш\, y) \\ &= x\left[y(y \,ш\, xy) + x(yy \,ш\, y)\right] + x\left[x(yy \,ш\, y) + yxyy\right] \\ &= x\left\{y\left[yxy + x(y \,ш\, y)\right] + x\left[y(y \,ш\, y) + yyy\right] + x\left[y(y \,ш\, y) + yyy\right] + yxyy\right\} \\ &= xyyxy + 2xyxyy + 3xxyyy + 3xxyyy + xyxyy \\ &= xyyxy + 3xyxyy + 6xxyyy \,. \end{aligned}$$

Note that although the shuffle product looks simpler for lack of a third term, it is generally much longer to compute than the stuffle counterpart. This is because the inductive definition is performed on each letter x, y rather than on z, of which there are fewer. So there is one less term per inductive step, but there are more inductive steps. In the example above we have $a = xyy = z_2 z_1$ and $b = xy = z_2$, so there are 5 letters x, y as opposed to 3 letters z. The difference is minimal, but already makes the calculation more cumbersome than the stuffle calculated in 2.2.12.

In general, there are only $l(\mathbf{a}) + l(\mathbf{b}) = r + s$ letters z as opposed to $wt(\mathbf{a}) + wt(\mathbf{b}) = a_1 + \ldots + a_r + b_1 + \ldots + b_s$ letters x, y.

Again, the shuffle product is aimed to replicate the product of MZVs when written as integrals. We make this precise as follows.

Definition 2.3.10. Define the map $Z^{ш} : \mathfrak{h}^0 \longrightarrow \mathbb{R}$ such that $Z^{ш}(x^{s_1-1}y \ldots x^{s_r-1}y) = \zeta(s_1, \ldots, s_n)$ and $Z^{ш}(1) = 1$, extended linearly to sentences.

Theorem 2.3.11. The map $Z^{ш} : (\mathfrak{h}^0, ш) \longrightarrow (\mathbb{R}, \cdot)$ is a $\mathbb{Q}$-algebra homomorphism.

Proof. The proof is almost identical to that for the stuffle product. Simply note that the shuffle product defined above has no 'third' term, for the latter corresponds to equating certain indices, which the integral will evaluate to 0. Proceed by induction on the sum of weights $n + m$, which is the sum of *lengths* on binary forms, and follow the same steps. □

Remark 2.3.12. This homomorphism also gives $(\mathcal{Z}, \cdot)$ an algebra structure, but no more than the stuffle product already provided.

Example 2.3.13. We decompose $\zeta(2,1)\zeta(2)$ into a linear combination of MZVs. The corresponding binary forms are $a = xyy$ and $b = xy$. By Example 2.3.9,

$$a \,ш\, b = xyyxy + 3xyxyy + 6xxyyy\,.$$

Using Theorem 2.3.11,

$$\begin{aligned} Z^{ш}(a \,ш\, b) &= Z^{ш}(xyyxy + 3xyxyy + 6xxyyy) \\ Z^{ш}(a)Z^{ш}(b) &= Z^{ш}(xyyxy) + 3Z^{ш}(xyxyy) + 6Z^{ш}(xxyyy) \\ \zeta(2,1)\zeta(2) &= \zeta(2,1,2) + 3\zeta(2,2,1) + 6\zeta(3,1,1)\,. \end{aligned}$$

Now comes the full power of stuffle and shuffle products. We have already expressed $\zeta(2,1)\zeta(2)$ as a linear combination of MZVs in Example 2.2.18, so we can compare both decompositions as follows:

$$\begin{aligned} & & \zeta(2,1)\zeta(2) &= \zeta(2,1)\zeta(2) \\ \Longrightarrow & & Z^{ш}(a \,ш\, b) &= Z^{*}(a * b) \\ \Longrightarrow & & \zeta(2,1,2) + 3\zeta(2,2,1) + 6\zeta(3,1,1) &= \zeta(2,1,2) + 2\zeta(2,2,1) + \zeta(2,3) + \zeta(4,1) \\ \Longrightarrow & & \zeta(2,2,1) + 6\zeta(3,1,1) &= \zeta(2,3) + \zeta(4,1)\,, \end{aligned}$$

giving us a highly non-trivial relation between MZVs.

Example 2.3.14. As a second example, we decompose $\zeta(2)\zeta(2)$ through stuffle and shuffle products. The binary forms are $a = xy = z_2 = b$, so we obtain

$$a * b = z_2z_2 + z_2z_2 + z_4 = 2z_2z_2 + z_4$$

and

$$a \,\text{ш}\, b = x(y \,\text{ш}\, xy) + x(xy \,\text{ш}\, y) = 2x\,[yxy + x(y \,\text{ш}\, y)] = 2xyxy + 4xxyy\,.$$

It now follows that

$$\begin{aligned} \zeta(2)\zeta(2) &= \zeta(2)\zeta(2) \\ Z^{\text{ш}}(a \,\text{ш}\, b) &= Z^{*}(a * b) \\ Z^{\text{ш}}(2xyxy + 4xxyy) &= Z^{*}(2z_2z_2 + z_4) \\ 2\zeta(2,2) + 4\zeta(3,1) &= 2\zeta(2,2) + \zeta(4,) \\ 4\zeta(3,1) &= \zeta(4) \end{aligned}$$

which is not *a priori* obvious, and involves only two MZVs. This is called a *double shuffle* relation, which comes from equating stuffle and shuffle products. We will later see that we can also obtain Euler's relation $\zeta(2,1) = \zeta(3)$ by extending this technique.

2.4 Double shuffle relations

We first note that $Z^{\text{ш}}$ and Z^{*} are really the same map:

$$Z^{\text{ш}}(x^{s_1-1}y\ldots x^{s_r-1}y) = Z^{\text{ш}}(z_{s_1}\ldots z_{s_n}) = \zeta(s_1,\ldots,s_n) = Z^{*}(z_{s_1}\ldots z_{s_n})\,,$$

so that we can write $Z = Z^{\text{ш}} = Z^{*}$. Using previous notation $\zeta(\mathbf{a}) = \zeta(\bar{\mathbf{a}})$, we can even write $\zeta = Z$. We only specify $*$ or ш to make precise which homomorphism we are talking about:

$$Z^{\text{ш}}(w \,\text{ш}\, w') = Z^{\text{ш}}(w)Z^{\text{ш}}(w') = \zeta(w)\zeta(w')$$

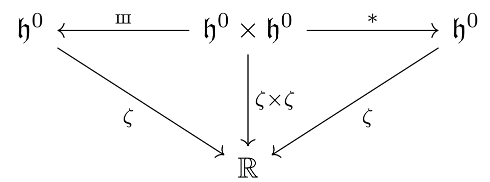
versus

$$Z^{*}(w * w') = Z^{*}(w)Z^{*}(w') = \zeta(w)\zeta(w')\,.$$

It follows immediately that

$$\zeta(w \,\text{ш}\, w') = \zeta(w)\zeta(w') = \zeta(w * w')\,,$$

which can be illustrated by the following commutative diagram.



This can be written in the following form.

Theorem 2.4.1 (Double shuffle relation)**.** For all words $w, w' \in \mathfrak{h}^0$,

$$\zeta(w \,\text{ш}\, w' - w * w') = 0\,.$$

Each choice of w, w' gives us a double shuffle (DS) relation, which is a linear relation among MZVs. This gives us infinitely many relations, as did the sum and cyclic sum theorems, this time arising from an elegant algebraic framework. Another crucial difference is that up to an extension process which we will now discuss, the DS is expected to produce *all* linear relations among MZVs. We make this precise as follows.

Given any $\mathbb{Q}$-relation between MZVs, we can move all terms to the LHS and multiply by the largest denominator to obtain a $\mathbb{Z}$-linear relation. We can write this as

$$\sum_{i \in I} \zeta(\mathbf{a}_i) = 0$$

for some finite indexing set I, and admissible multi-indices $\mathbf{a}_i$. Equivalently, we can write $w = \sum_{i \in I} \bar{\mathbf{a}}_i \in \mathfrak{h}^0$ to obtain the equivalences:

$$\sum_{i \in I} \zeta(\mathbf{a}_i) = 0 \iff \sum_{i \in I} \zeta(\bar{\mathbf{a}}_i) = 0 \iff \zeta\left(\sum_{i \in I} \bar{\mathbf{a}}_i\right) = 0 \iff w \in \ker(\zeta)$$

when viewing ζ as the map $\zeta = Z : \mathfrak{h}^0 \longrightarrow \mathbb{R}$ as usual. In this language, the double shuffle relation states that

$$w \sqcup\!\sqcup\, w' - w * w' \in \ker(\zeta)$$

for all $w, w' \in \mathfrak{h}^0$. Inspired from Henderson in [Hen, Chap. 3], let $\mathcal{D} := \{w \sqcup\!\sqcup\, w' - w * w' \mid w, w' \in \mathfrak{h}^0\}$. Then we can write

$$\mathcal{D} \subseteq \ker(\zeta)\,.$$

To say that the double shuffle produces all linear relations between MZVs would be equivalent to saying $\mathcal{D} \supseteq \ker(\zeta)$ or $\mathcal{D} = \ker(\zeta)$. This is not true, as the following proposition makes explicit.

Proposition 2.4.2. Euler's relation $\zeta(2, 1) = \zeta(3)$ cannot be obtained from the DS relations.

The basic idea of the proof is that weight is respected in a particular way by the DS. If we could find $w, w' \in \mathfrak{h}^0$ such that $w \sqcup\!\sqcup\, w' - w * w' = \zeta(2, 1) - \zeta(3)$, then one of w or w' would need to have weight 1 since the products have weight $3 = wt(w) + wt(w')$. But there are no MZVs of this weight, so this cannot happen.

Remark 2.4.3. The crucial element of the above proposition is that we take $u, v \in \mathfrak{h}^0$. This forces the weights of non-identity words in u, v to be ≥ 2, so that any stuffle or shuffle product will be of weight ≥ 4. But Euler's relation is in weight 3, which renders it inaccessible.

If we could take $u, v \in \mathfrak{h}^1$ instead, the weights only need to be ≥ 1, so that relations of weight 3 could be obtained. The problem is that the map $\zeta : \mathfrak{h}^0 \longrightarrow \mathbb{R}$ does not extend to $\mathfrak{h}^1$, since a word of weight 1 (which can only be $y \in \mathfrak{h}^1$) would be sent to infinity: $\zeta(y) = \zeta(z_1) = \zeta(1) = \infty \notin \mathbb{R}$. If we could extend the map to the image $\mathbb{R} \cup \{\infty\}$ and work with infinities, one could obtain Euler's relation in the following way. Take $a = y = z_1$, $b = xy = z_2$. Then

$$\begin{aligned} a \sqcup\!\sqcup\, b &= y(1 \sqcup\!\sqcup\, xy) + x(y \sqcup\!\sqcup\, y) = yxy + 2xyy = z_1 z_2 + 2 z_2 z_1 \\ a * b &= z_1 z_2 + z_2 z_1 + z_3 \end{aligned}$$

which implies $a ⧢ b - a * b = z_2 z_1 - z_3 \in \mathfrak{h}^0$. We obtain

$$\zeta(a ⧢ b - a * b) = \zeta(z_2 z_1 - z_3) = \zeta(2,1) - \zeta(3)\,.$$

Now note that $\zeta(1) = \infty$ (the series diverges). If we could make the cancellation $\zeta(1) - \zeta(1) = 0$ (which is not allowed!), then

$$\zeta(a ⧢ b - a * b) = \zeta(a)\zeta(b) - \zeta(a)\zeta(b) = (\zeta(1) - \zeta(1))\zeta(2) = 0\,,$$

giving Euler's relation. This naïve cancelling of divergent series breaches the rules of arithmetic (the indeterminate form $\infty - \infty$ is ill-defined), but Ihara-Kaneko-Zagier have found a way to perform a similar operation rigorously in [IKZ]. Their work extends the double shuffle to produce relations which come from divergent series, including Euler's relation. The process is called *regularisation*, and the extended double shuffle (EDS) is expected to produce *all* linear relations between MZVs.

Remark 2.4.4. This form of regularisation is not to be confused with *renormalisation*, a technique to control infinities by "adjusting for self-interaction feedback" (Wikipedia), whose tools are mostly applied in physics.

It is also not to be confused with zeta function regularisation, which assigns finite values to divergent sums through analytic continuation of the Riemann zeta function - in particular the infamous

$$\zeta(-1) = 1 + 2 + 3 + 4 + \ldots = -1/12\,.$$

It *does* however resemble Martin Hairer's work on regularity structures (c.f. [Hai]) in the area of stochastic PDEs, in which an analogous notion of 'cancelling infinities' can be found. I was lucky to attend one of his talks last year, and asked him about whether his procedure is similar in nature to ours. He said that the underlying idea is essentially the same, and can in fact be viewed algebraically – although the methods involved are very different.

He has now written a paper [BHZ] with Bruned and Zambotti named *Algebraic renormalisation of regularity structures*, involving Hopf algebras of "decorated coloured forests". This is strangely similar in name to Goncharov's "Hopf algebra of decorated rooted plane trivalent trees" (whose paper [Gon] we will invoke in Chapter 5), although there is most likely no relation at all here, and we are going far beyond the subject of this report!

2.5 Regularisation and the extended double shuffle

We refer the reader to [IKZ] for a full exposition of regularisation. Although beautiful and interesting in its own right, the work of IKZ involves some amount of notation and technicalities which lead astray from this report's purpose. In this section I develop a simple way of understanding the main result, explain its significance and foreshadow an algebraic approach to some of this extension process.

My formulation is simple and intuitive, but gives no insight into the proof. We recommend the reader to read this section and proceed to IKZ's paper if interested.

Definition 2.5.1. Define the 'filtering' function $f : (\mathfrak{h}^1, *) \longrightarrow (\mathfrak{h}^0, *)$ as the algebra homomorphism which extends the identity map $I : \mathfrak{h}^0 \longrightarrow \mathfrak{h}^0$ and sends $y = z_1$ to 0. More precisely,

$$f(w) = \begin{cases} w & \text{if } w \in \mathfrak{h}^0 \\ 0 & \text{if } w = y \end{cases}$$

and $f(u * v) = f(u) * f(v)$ for all $u, v \in \mathfrak{h}^1$.

For this function to be well-defined, we need to show that any word $w \in \mathfrak{h}^1$ can be written as a 'polynomal' in y with elements in $\mathfrak{h}^0$ as sentences, where the polynomial product is the stuffle $*$. The proof of this can be found in [BGF] by induction on length. This implies that any word $w \in \mathfrak{h}^1$ can be written as

$$\sum_{i=0}^{n} w_i * \underbrace{y * \ldots * y}_{i \text{ times}}$$

with $w_i \in \mathfrak{h}^0$. Since f is a linear homomorphism, this implies

$$f(w) = \sum_{i=0}^{n} f(w_i) f(y)^i = w_0 \,,$$

which defines f uniquely for all $w \in \mathfrak{h}^1$, as required for the definition to make sense.

Example 2.5.2. Let $w = z_1 z_2 \in \mathfrak{h}^1 \setminus \mathfrak{h}^0$. Then

$$w = z_1 * z_2 - z_2 z_1 - z_3 = y * z_2 - z_2 z_1 - z_3 \,,$$

which expresses w as an $*$-polynomial in y with $w_1 = z_2$ and $w_0 = -z_2 z_1 - z_3$. As a result,

$$f(w) = f(y) f(z_2) - f(z_2 z_1) - f(z_3) = -z_2 z_1 - z_3 = w_0 \,.$$

Note that this function allows us to extend $\zeta : \mathfrak{h}^0 \longrightarrow \mathbb{R}$ to $\zeta \circ f : \mathfrak{h}^1 \longrightarrow \mathbb{R}$. For our purposes, the work of IKZ can be summarised by the following result, which is a corollary to [IKZ, Th. 1]. Much more than a corollary, it is equivalent to Theorem 1 by part $(i) \iff (iv)$ of Theorem 2 in the same paper, where f is written as reg_*.

Theorem 2.5.3 (EDS)**.** For all $w_0 \in \mathfrak{h}^0$ and $w_1 \in \mathfrak{h}^1$,

$$\zeta \circ f(w_0 \,ш\, w_1 - w_0 * w_1) = 0 \,.$$

Remarks 2.5.4.

1. This is well-defined since $w_0, w_1 \in \mathfrak{h}^1 \implies w_0 \,ш\, w_1, w_0 * w_1 \in \mathfrak{h}^1$, an easy exercise by induction on the sum of word lengths.
2. This theorem would hold immediately if $\zeta \circ f : (\mathfrak{h}^1, *) \longrightarrow (\mathbb{R}, \cdot)$ and $\zeta \circ f : (\mathfrak{h}^1, ш) \longrightarrow (\mathbb{R}, \cdot)$ were *both* algebra homomorphisms. $\zeta \circ f$ is a homomorphism with respect to the stuffle since both ζ and f are, but the claim fails for the shuffle. Taking $a = y, b = y$ gives

$$\zeta \circ f(a \,ш\, b) = \zeta \circ f(2yy) = \zeta \circ f(z_1 * z_1 - z_2) = \zeta(-z_2) = -\zeta(2) \,,$$

whereas

$$\zeta \circ f(a) \cdot \zeta \circ f(b) = \zeta(0) \cdot \zeta(0) = 0 \cdot 0 = 0 \,.$$

These are not equal since $\zeta(2) = \pi^2/6 > 0$.

3. For $w_1 \in \mathfrak{h}^0$ we have $w_0 ш w_1, w_0 * w_1 \in \mathfrak{h}^0$, so $f(w_0 ш w_1 - w_0 * w_1) = w_0 ш w_1 - w_0 * w_1$ and the result reduces to
$$\zeta(w_0 ш w_1 - w_0 * w_1) = 0\,,$$
the double shuffle relation.

4. For $w_1 \notin \mathfrak{h}^0$, we may still have $w_0 ш w_1 - w_0 * w_1 \in \mathfrak{h}^0$ if the words in $\mathfrak{h}^1$ cancel. Then the theorem looks exactly like the double shuffle above. However we cannot use the standard DS to obtain the result by writing
$$\zeta(w_0 ш w_1 - w_0 * w_1) = \zeta(w_0 ш w_1) - \zeta(w_0 * w_1) = \zeta(w_0)\zeta(w_1) - \zeta(w_0)\zeta(w_1) = 0\,,$$
since $\zeta(w_1)$ is not even defined for $w_1 \notin \mathfrak{h}^0$. Even if we defined $\zeta(w_1) = \zeta(1, \ldots) = \infty$ (words in $\mathfrak{h}^1 \setminus \mathfrak{h}^0$ begin with z_1, and the series diverges), the last equality would require cancelling infinities $\infty - \infty = 0$, as previously foreshadowed. The theorem allows us to overcome this difficulty. Indeed, recalling our attempt to produce Euler's relation, take $w_0 = xy = z_2$ and $w_1 = z_1 \notin \mathfrak{h}^0$. We have
$$w_0 ш w_1 - w_0 * w_1 = z_1z_2 + 2z_2z_1 - z_1z_2 - z_2z_1 - z_3 = z_2z_1 - z_3 \in \mathfrak{h}^0\,,$$
and the theorem gives us Euler's relation
$$\zeta(z_2z_1 - z_3) = 0 = \zeta(2,1) - \zeta(3)\,.$$

5. Taking f to be a homomorphism with respect to the stuffle product instead of the shuffle was an arbitrary choice. The choices are shown to be equivalent in [IKZ], but the reader may prefer one over the other in terms of computational ease.

We define the extended double shuffle (EDS) relations to be those produced from the theorem above. Letting $\overline{\mathcal{D}} = \{f(w_0 ш w_1 - w_0 * w_1) \mid w_0 \in \mathfrak{h}^0, w_1 \in \mathfrak{h}^1\} \subset \mathfrak{h}^0$, the theorem states that
$$\overline{\mathcal{D}} \subseteq \ker(\zeta)\,.$$
Taking $w_1 \in \mathfrak{h}^0$ gives the DS by the third remark, so $\mathcal{D} \subseteq \overline{\mathcal{D}}$. By the fourth remark and Proposition 2.4.2, we have strict inclusion $\mathcal{D} \subset \overline{\mathcal{D}}$. The conjecture below states that the EDS produces all linear relations among MZVs; [IKZ, p. 315] states that it has been checked numerically "up to weight 16 by Minh, Petiot *et al.* in Lille". One can think of the EDS as the *completion* of the DS, in such a way that we obtain every possible relation.

Conjecture 2.5.5. $\overline{\mathcal{D}} = \ker(\zeta)\,.$

In fact, a stronger result is conjectured to hold. Instead of taking the full set of EDS relations, we will take a small subset called Hoffman's relation (first discovered in [Hof1] with different notation), along with the DS.

Theorem 2.5.6 (Hoffman's relation)**.** For all $w_0 \in \mathfrak{h}^0$,
$$\zeta(w_0 ш y - w_0 * y) = 0\,.$$

Up to omitting the function f, this is the EDS with $w_1 = y \in \mathfrak{h}^1$. If we can show that $w_0 ш y - w_0 * y$ is in $\mathfrak{h}^0$, then

$$f(w_0 ш y - w_0 * y) = w_0 ш y - w_0 * y$$

and Hoffman's relation will indeed be a corollary to the EDS. The following proposition establishes exactly this.

Proposition 2.5.7. For any $w_0 \in \mathfrak{h}^0$,

$$w_0 ш y - w_0 * y \in \mathfrak{h}^0 .$$

Proof. Write

$$w_0 = \sum_{i \in I} p_i w_i$$

for some finite indexing set I with $0 \neq p_i \in \mathbb{Q}$ and words $0 \neq w_i \in \mathfrak{h}^0$. We prove the claim for each w_i, which will prove the proposition since

$$w_0 ш y - w_0 * y = \sum_{i \in I} p_i (w_i ш y - w_i * y)$$

and $\mathfrak{h}^0$ is a $\mathbb{Q}$-vector space. If $w_i = 1$ then $1 ш y - 1 * y = y - y = 0 \in \mathfrak{h}^0$ so we are done. Otherwise, write $w_i = z_{a_1} \dots z_{a_r} = z_{a_1} u$ with $r \geq 1$, $a_1 \geq 2$, $u \in \mathfrak{h}^1$. Then

$$\begin{aligned} w_i ш y - w_i * y &= x(z_{a_1 - 1} u ш y) + y(w_i ш 1) - z_{a_1}(u * y) - z_1(w_i * 1) - z_{a_1+1}(u * 1) \\ &= x(z_{a_1 - 1} u ш y) - z_{a_1}(u * y) - z_{a_1+1} u \\ &= x \left[z_{a_1 - 1} u ш y - z_{a_1 - 1}(u * y) - z_{a_1} u \right] . \end{aligned}$$

Now $u, y \in \mathfrak{h}^1 \implies u ш y, u * y \in \mathfrak{h}^1$, so the element inside the square bracket is in $\mathfrak{h}^1$. Therefore x times that element is in $\mathfrak{h}^0$, and we are done. □

Define $\mathcal{H} = \{ w_0 ш y - w_0 * y \mid w_0 \in \mathfrak{h}^0 \}$. By the proposition above,

$$\mathcal{H} \subseteq \overline{\mathcal{D}} \subseteq \ker(\zeta) .$$

We have also shown that $\mathcal{D} \subset \overline{\mathcal{D}}$, so we have

$$\mathcal{D} \cup \mathcal{H} \subseteq \overline{\mathcal{D}} \subseteq \ker(\zeta) .$$

The conjecture, also verified numerically up to weight 16, is that the DS and Hoffman's relation produce all linear relations among MZVs, as follows.

Conjecture 2.5.8. $\mathcal{D} \cup \mathcal{H} = \ker(\zeta)$.

One may ask what is the purpose of using Hoffman's relation (HR) instead of the full EDS, of which it is a corollary. The first answer is that HR is much simpler than the full EDS, and does not involve the function f, so we do not need to filter words in $\mathfrak{h}^1$. The more profound answer is that HR can be proved with purely algebraic methods, as opposed to regularisation which involves analytic procedures described in [IKZ].

Before moving to the next chapter, we return to the question of dimension posed in Section 1.4. If we can count the number of independent relations that DS and HR produce in weight k, we will obtain an upper bound on dimension by subtracting it from 2^{k-2}. Moreover, Conjecture 2.5.8 would imply that this upper bound is reached, i.e. equals $\dim_{\mathbb{Q}}(Z_k)$.

The issue is that we may be able to count the number of relations they produce, but it is hard to determine whether any given relations are independent, i.e. whether one cannot be obtained as a linear combination of others. As a result, we do not obtain any relevant result on general dimension, and the results of Terasoma, Deligne-Goncharov and Brown involve (much) more advanced machinery. However, we can still obtain upper bounds for low weights by working through all possibilities, illustrated below.

Example 2.5.9. We prove that $\dim(\mathcal{Z}_4) \leq 1 = d_4$ using HR and DS. In the particular case that $d_k = 1$, we actually obtain equality since the space is non-empty (MZVs are not zero). In general this method would only give an upper bound, since proving linear independence is out of reach for now. First note that there are $2^2 = 4$ MZVs of weight 4: $\zeta(4), \zeta(3,1), \zeta(2,2)$ and $\zeta(2,1,1)$.

First note that Example 2.3.14 already establishes

$$4\zeta(3,1) = \zeta(4)$$

by using the DS, which eliminates $\zeta(3,1)$ and gives $\dim(\mathcal{Z}_4) \leq 3$. We now use Hoffman's relation with $w_0 = xxy = z_3$. First compute the shuffle and stuffle products,

$$\begin{aligned} w_0 \sqcup\!\sqcup\, y &= x(xy \sqcup\!\sqcup\, y) + yxxy \\ &= x\left[x(y \sqcup\!\sqcup\, y) + yxy\right] + yxxy \\ &= 2xxyy + xyxy + yxxy \\ &= 2z_3z_1 + z_2z_2 + z_1z_3 \end{aligned}$$

and

$$\begin{aligned} w_0 * y &= z_3 * z_1 \\ &= z_3z_1 + z_1z_3 + z_4\,. \end{aligned}$$

By Hoffman's relation,

$$\begin{aligned} \zeta(z_3z_1 + z_2z_2 - z_4) &= 0 \\ \zeta(3,1) + \zeta(2,2) &= \zeta(4) \end{aligned}$$

and we use $4\zeta(3,1) = \zeta(4)$ to obtain

$$\zeta(2,2) = \frac{3}{4}\zeta(4)\,.$$

This reduces the dimension by one again. Again, use Hoffman's relation with $w_0 = xyy = z_2z_1$. We have

$$\begin{aligned} w_0 \sqcup\!\sqcup\, y &= x(yy \sqcup\!\sqcup\, y) + yxyy \\ &= x\left[y(y \sqcup\!\sqcup\, y) + yyy\right] + yxyy \\ &= 3xyyy + yxyy \\ &= 3z_2z_1z_1 + z_1z_2z_1 \end{aligned}$$

and

$$\begin{aligned} w_0 * y &= z_2(z_1 * z_1) + z_1 z_2 z_1 + z_3 z_1 \\ &= 2 z_2 z_1 z_1 + z_2 z_2 + z_1 z_2 z_1 + z_3 z_1 \,. \end{aligned}$$

Using the previous relations and Hoffman's relation, we obtain

$$\zeta(2,1,1) = \zeta(2,2) + \zeta(3,1) = \zeta(4) \,.$$

We have expressed all MZVs of weight 4 in terms of $\zeta(4)$, so we obtain $\mathcal{Z}_4 = \{c\zeta(4) \mid c \in \mathbb{Q}\}$ with $\dim(\mathcal{Z}_4) = 1$. This would not have been possible with the double shuffle alone!

The next chapter introduces concepts including derivations, building towards Hoffman's relation. This provides us with a fully algebraic framework expected to generate all relations among MZVs.

Chapter 3

Duality, derivations and Ohno's Theorem

3.1 Duality

Before going into the topic of derivations we work towards the duality theorem, a family of relations equating (almost) any MZV to another, thus 'folding' the space in two. It takes root in the integral formulation for MZVs, where a certain change of variable can be applied. This is both beautiful in itself and will be used in the next section to state Hoffman's relation.

Definition 3.1.1. Define the endomorphism $\tau : \mathfrak{h} \longrightarrow \mathfrak{h}$ by $\mathbb{Q}$-linear extension of

$$\tau(x) = y \qquad \tau(1) = 1$$
$$\tau(y) = x \qquad \tau(ab) = \tau(b)\tau(a)$$

for any words $a, b \in \mathfrak{h}$.

It follows from definition that $\tau^2(w) = w$ for all $w \in \mathfrak{h}$, so that τ is an automorphism with $\tau^{-1} = \tau$.

Proposition 3.1.2. The map τ preserves weight and 'inverts' length, that is,

$$wt(w) = n \quad \Longrightarrow \quad wt(\tau(w)) = n$$
$$l(w') = r \quad \Longrightarrow \quad l(\tau(w')) = n - r$$

for all words $w \in \mathfrak{h}$, $w' \in \mathfrak{h}^1$ (for length to be defined).

Proof. Write $w = \epsilon_1 \ldots \epsilon_n$ with $\epsilon_i \in \{x, y\}$. Then $\tau(w) = \tau(\epsilon_n) \ldots \tau(\epsilon_1)$, so that $wt(\tau(w)) = n = wt(w)$. If moreover $w \in \mathfrak{h}^1$, write $w = z_{i_1} \ldots z_{i_r}$. Then

$$\tau(w) = xy^{i_r - 1} \ldots xy^{i_1 - 1}$$

which has $i_1 + \ldots + i_r - r = n - r$ letters y, so that $l(\tau(w)) = n - r = wt(w) - l(w)$. $\square$

Theorem 3.1.3 (Duality)**.** For any word $w \in \mathfrak{h}^0$,

$$\zeta(\tau(w)) = \zeta(w)\,.$$

The duality theorem is strikingly elegant, and comes from a simple change of variables in the integral formulation of MZVs. The proof is given in Appendix A.3.

Examples 3.1.4.

1. Take $w = xyy = z_2z_1$. Then $\tau(w) = \tau(y)\tau(xy) = x\tau(y)\tau(x) = xxy = z_3$, so that
$$\zeta(2,1) = \zeta(w) = \zeta(\tau(w)) = \zeta(3)\,,$$
i.e. duality implies Euler's relation.

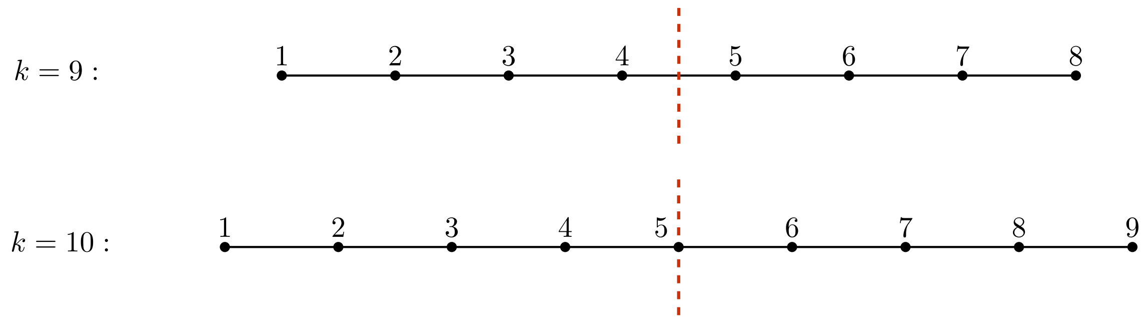
2. Take $w = xyyy$, then $\tau(w) = xxxy$ gives us
$$\zeta(2,1,1) = \zeta(4)\,,$$
which agrees with the length-reversing property: $l(\tau(w)) = 1 = 4 - 3 = wt(w) - l(w)$.

3. Attempting to bound the dimension of $\mathcal{Z}_4 = \text{span}\{\zeta(4), \zeta(3,1), \zeta(2,2), \zeta(2,1,1)\}$, we can try to use the duality theorem on all of the corresponding words in $\mathfrak{h}^0$. The above example shows that $\zeta(4)$ and $\zeta(2,1,1)$ are dual, so let us check the other two. For $w = z_3z_1 = xxyy$ we have $\tau(w) = xxyy = w$, giving us the tautology
$$\zeta(3,1) = \zeta(3,1)\,.$$
Similarly $w = z_2z_2 = xyxy$ gives $\tau(w) = xyxy = w$. So in total, the duality theorem only gives us $\dim \mathcal{Z}_4 \leq 3$. We know that $\dim \mathcal{Z}_4 = 1$, so the duality theorem does not give us all $\mathbb{Q}$-linear relations, but remains a powerful and elegant result.

Remark 3.1.5. Duality is slightly powerful in producing relations in odd weight. Indeed, the length-reversing property insures that $l(\tau(w)) = wt(w) - l(w) = n - l(w)$. For n odd, this gives us $l(\tau(w)) \neq l(w)$ since otherwise, $2l(w) = n$, a contradiction. Thus every multi-index is not self-dual in odd weight.

On the contrary, we may have self-dual multi-indices for even weight, as has been shown for $(3,1)$ and $(2,2)$ in $\mathcal{Z}_4$. These self-dual elements must occur exactly at $l(w) = n/2$ by the above reasoning, which is indeed the case here: $l(2,2) = l(3,1) = 2 = 4/2$.

This is what we mean by the initial statement that duality equates 'almost' any MZV to another: it does so in odd weight, and does so for all words not of length $n/2$ in even weight. This (almost) folds the space in two, with length as symmetry:



The number of MZVs of fixed weight $k \geq 2$ is 2^{k-2} by Proposition 1.4.6, and we obtain the following result.

Corollary 3.1.6. For all $k \geq 3$, we have

$$\dim(\mathcal{Z}_k) \leq \begin{cases} 2^{k-3} & \text{if } k \text{ is odd} \\ 2^{k-3} + \frac{1}{2}\binom{k-2}{k/2-1} & \text{if } k \text{ is even.} \end{cases}$$

Proof. In Appendix A.3, including two different proofs for k odd and a more elegant proof of Proposition 1.4.6. □

Note that the bound is not optimal for k even, since *some* MZVs on the symmetric strip $k/2$ *are* self-dual, while others are not. For example, taking $w = xxyyxy$ in weight 6, length 3 gives duality

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

which eliminates $\zeta(3,1,2)$. We give a few easy exercises that we have solved ourselves, for the reader who wants to refine this bound further. We will not spend more time on this or give solutions, for it diverges from the purpose of this chapter.

Exercises 3.1.7. Let k even and $\mathbf{a} = (a_1, \dots, a_r)$ of length $r = k/2$.

1. Prove that $\mathbf{a}$ is not self-dual if $a_i \geq 3$ for all i.
2. Prove that $\mathbf{a}$ is not self-dual if $a_1 = 2$ and $a_r = 1$.
3. Prove that $\mathbf{a}$ is not self-dual if $a_1 > 2$ and $a_r > 1$.

3.2 Derivations

In this section we follow Hoffman-Ohno in [HO].

Definition 3.2.1. A derivation of $\mathfrak{h}$ is a $\mathbb{Q}$-linear map $F : \mathfrak{h} \longrightarrow \mathfrak{h}$ such that

$$F(uv) = F(u)v + uF(v)$$

for all $u, v \in \mathfrak{h}$.

By defining

$$(aF + bG)(w) = aF(w) + bG(w)$$

for derivations F, G, rationals $a, b \in \mathbb{Q}$, and words $w \in \mathfrak{h}$, the set of derivations forms a vector space over $\mathbb{Q}$, which we name $\mathrm{Der}(\mathfrak{h})$. We will not use the following proposition, but state it as an interesting fact in its own right.

Proposition 3.2.2. The space $\mathrm{Der}(\mathfrak{h})$ is a Lie algebra with Lie bracket $[F, G] = FG - GF$.

Proof. The definition of a Lie algebra is a vector space endowed with a non-associative "Lie bracket" such that $[F, G] \in \mathrm{Der}(\mathfrak{h})$ for all $F, G \in \mathfrak{h}$. It remains only to prove the latter. For all words $a, b \in \mathfrak{h}$, we have

$$\begin{aligned}
[F, G]\,(ab) &= F(aG(b) + G(a)b) - G(aF(b) + F(a)b) \\
&= F(a)G(b) + aFG(b) + FG(a)b + G(a)F(b) \\
&\quad - G(a)F(b) - aGF(b) - GF(a)b - F(a)G(b) \\
&= aFG(b) - aGF(b) + FG(a)b - GF(a)b \\
&= a\,[F, G]\,(b) + [F, G]\,(a)b
\end{aligned}$$

as required to be part of $\mathrm{Der}(\mathfrak{h})$. □

One can view derivations as the algebraic counterpart of derivatives in calculus (ordinary or partial), which indeed satisfy the property

$$\frac{d}{dx}(f \cdot g) = \frac{d}{dx}(f) \cdot g + f \cdot \frac{d}{dx}(g)$$

for appropriate functions, say $f, g : \mathbb{R} \longrightarrow \mathbb{R}$. This is usually called the 'product rule'. This trivially extends to any number of products, namely

$$F(u_1 \ldots u_n) = F(u_1)u_2 \ldots u_n + \ldots + u_1 \ldots u_{n-1}F(u_n)$$

for all $u_i \in \mathfrak{h}$, $n \in \mathbb{N}$.

Note that taking $u = v = 1$ we obtain

$$F(1) = F(1) + F(1) \implies F(1) = 0\,,$$

which mirrors the idea that differentiating a constant gives 0.

Proposition 3.2.3. If F is a derivation then so is $\bar{F} = \tau F \tau$.

The proof is left as an easy exercise.

Definition 3.2.4. Define the standard derivation $D : \mathfrak{h} \longrightarrow \mathfrak{h}$ such that

$$D(x) = 0 \quad \text{and} \quad D(y) = xy\,.$$

Note that this is a derivation *by definition*, i.e. we define it to satisfy the properties above along with $D(uv) = D(u)v + uD(v)$. Then we also obtain the derivation $\bar{D}$, satisfying

$$\bar{D}(x) = \tau(D(y)) = \tau(xy) = xy \qquad \text{and} \qquad \bar{D}(y) = \tau(D(x)) = 0\,.$$

We will often abuse notation by writing $Fu = F(u)$ for derivations F.

Example 3.2.5.

$$D(z_3) = D(xxy) = D(xx)y + xxD(y) = D(x)xy + xD(x)y + xxxy = xxxy = z_4$$

$$\bar{D}(z_3) = \bar{D}(xx)y + xx\bar{D}(y) = \bar{D}(x)xy + x\bar{D}(x)y + xx\bar{D}(y) = xyxy + xxyy = z_2z_2 + z_3z_1$$

The following lemma generalises this example, allowing us to view D as acting on each letter z_n of a word separately and uniformly (increasing n by 1), whereas $\bar{D}$ acts as in a more subtle way, as a convolution. This can be thought of as reflecting the stuffle and shuffle products respectively: the former is defined on letters z, whereas the latter requires the finer x, y presentation.

Lemma 3.2.6. For any $k \in \mathbb{N}$,

$$D(z_k) = z_{k+1} \qquad \text{and} \qquad \bar{D}(z_k) = \sum_{n=1}^{k-1} z_{n+1} z_{k-n} \,.$$

Proof. By product rule we have

$$D(z_k) = D(x)z_{k-1} + \ldots + x^{k-1}D(y) = 0 + \ldots + 0 + x^{k-1}xy = z_{k+1}$$

and

$$\bar{D}(z_k) = \bar{D}(x)z_{k-1} + \ldots + x^{k-1}\bar{D}(y) = z_2 z_{k-1} + \ldots + z_k z_1 + 0 = \sum_{n=1}^{k-1} z_{n+1} z_{k-n} \,.$$

□

Following definition, it is immediate to see that $D(\mathfrak{h}^0), \bar{D}(\mathfrak{h}^0) \subset \mathfrak{h}^0$. This implies that the following theorem is well-defined, and is due to Hoffman.

Theorem 3.2.7. For all words $w \in \mathfrak{h}^0$,

$$\zeta(Dw) = \zeta(\bar{D}w) \,.$$

We can also write this as $\zeta(Dw - \bar{D}w) = 0$. The proof is given in [Hof1, Theorem 5.1] or in [Ohn, Theorem 1 with $l = 1$]. The former uses partial fractions while the latter involves a change of variables in the integral formulation, albeit much more sophisticated than that which we used to prove duality. Both proofs are left out for they are a little complicated, but remain 'elementary' and rest purely on algebraic manipulation.

Example 3.2.8. Taking $w = xy$ gives

$$\begin{aligned} Dw &= D(x)y + xD(y) = xxy \\ \bar{D}w &= \bar{D}(x)y + x\bar{D}(y) = xyy \,. \end{aligned}$$

Then the theorem gives us Euler's relation

$$\zeta(3) = \zeta(Dw) = \zeta(\bar{D}w) = \zeta(2,1) \,.$$

Now comes the usefulness of derivations in proving Hoffman's relation algebraically, which conjecturally replaces our need for the analytic process of regularisation.

Proposition 3.2.9. For all $w \in \mathfrak{h}^1$,

$$w \sqcup\!\sqcup\, y - w * y = \bar{D}w - Dw \,.$$

This appears as Theorem 4.3 in [HO], but I have not read their proof. I would expect it to be similar to mine, given below. With this result in hand along with Theorem 3.2.7, we obtain Hoffman's relation:

$$\zeta(w \sqcup\!\sqcup y - w * y) = \zeta(\bar{D}w - Dw) = 0\,.$$

Proof. As usual, proving this for any word $w \in \mathfrak{h}^1$ induces the full result. We proceed by induction on the length of w. For $l(w) = 0$ we have $w = 1$, whereby

$$1 \sqcup\!\sqcup y - 1 * y = 0 = \bar{D}(1) - D(1)\,.$$

Assume the claims holds for all $k \leq r - 1$, and take $w = z_{a_1} \dots z_{a_r} = z_{a_1} u \in \mathfrak{h}^0$. Then

$$\begin{aligned} w \sqcup\!\sqcup y - w * y &= x(z_{a_1-1} u \sqcup\!\sqcup y) + yw - z_{a_1}(u * y) - yw - z_{a_1+1} u \\ &= x^2(z_{a_1-2} u \sqcup\!\sqcup y) + z_2 z_{a_1-1} u - z_{a_1}(u * y) - z_{a_1+1} u \\ &\quad \vdots \\ &= z_{a_1}(u \sqcup\!\sqcup y) + \sum_{n=1}^{a_1-1} z_{n+1} z_{a_1-n} u - z_{a_1}(u * y) - z_{a_1+1} u \\ &= z_{a_1}(\bar{D}u - Du) + \bar{D}(z_{a_1})u - D(z_{a_1})u \\ &= z_{a_1}\bar{D}(u) + \bar{D}(z_{a_1})u - z_{a_1}D(u) - D(z_{a_1})u \\ &= \bar{D}(w) - D(w)\,. \end{aligned}$$

□

Since both the above proposition and Theorem 3.2.7 are proved algebraically, it follows that Hoffman's relation can be viewed equally well as an algebraic result, as opposed to a corollary of regularisation. Finally, under the conjecture stating that

$$\mathcal{D} \cup \mathcal{H} = \ker(\zeta)\,,$$

we expect that all relations between MZVs are produced by DS and HR, avoiding regularisation entirely. In my opinion, the limitation of such a bypass resides in the proof of Theorem 3.2.7, which is not particularly appealing to me. The reader can choose for themselves which they prefer, but should keep in mind that they are conjecturally equivalent.

The next sections give a much more satisfying understanding of this equivalence, which up to now has been numerical. We expose Ohno's Theorem and the derivation relations, a particular case of which is Hoffman's relation, and state IKZ's result that they are fully equivalent to the EDS (not numerically but algebraically!).

3.3 Ohno's Theorem

Ohno's Theorem is a large family of relations first formulated by Ohno in [Ohn, Theorem 1]. In this section we present the result in its elegant re-formulation as given in [HO]. We must first define the notion of a coproduct, and for completeness we mention that this turns $\mathfrak{h}^1$ into a Hopf algebra, without detail or proof.

Definition 3.3.1. Define the $\mathbb{Q}$-linear coproduct $\Delta : \mathfrak{h}^1 \longrightarrow \mathfrak{h}^1 \otimes \mathfrak{h}^1$ as

$$\Delta(z_{a_1} \dots z_{a_r}) = \sum_{j=0}^{r} z_{a_1} \dots z_{a_j} \otimes z_{a_{j+1}} \dots z_{a_r}$$

where $z_{a_0} = z_{a_{r+1}} := 1$.

Example 3.3.2. For $w = z_1 + z_2 z_3$ we obtain

$$\Delta(w) = \Delta(z_1) + \Delta(z_2 z_3) = 1 \otimes z_1 + z_1 \otimes 1 + 1 \otimes z_2 z_3 + z_2 \otimes z_3 + z_2 z_3 \otimes 1\,.$$

This coproduct (with appropriate choices of unit, co-unit and antipode) turn the algebra $(\mathfrak{h}^1, *)$ into a Hopf algebra $(\mathfrak{h}^1, *, \Delta)$ isomorphic to QSym, the quasi-symmetric functions. We will not use this further algebraic structure in this report, so we leave the statement with neither explanation of what a Hopf algebra is, nor proof. For a very detailed exposition of this subject, we refer the reader to [Hen, Chapters 4,5].

Definition 3.3.3 (Following OH)**.** Define the bilinear map $\cdot : \mathfrak{h}^1 \otimes \mathfrak{h}^1 \longrightarrow \mathfrak{h}^1$ by the following. First we take $1 \cdot w = w$ for any word $w \in \mathfrak{h}^1$. For any $1 \neq u \in \mathfrak{h}^1$, let $u \cdot x = 0$ and

$$u \cdot y = \begin{cases} z_{k+1} & \text{if } u = z_k \\ 0 & \text{otherwise} \end{cases}.$$

For all words $w_1, w_2 \in \mathfrak{h}^1$, define

$$u \cdot w_1 w_2 = \sum_{u_1 \otimes u_2 \in \Delta(u)} (u_1 \cdot w_1)(u_2 \cdot w_2)$$

where $\Delta(u) = \sum u_1 \otimes u_2$.

Remarks 3.3.4.

1. This is not to be confused with concatenation $\cdot$, which we always leave implicit.

2. For the interested reader, this map is moreover an algebra action of $\mathfrak{h}^1$ on $\mathfrak{h}^1$, which will be a consequence of proposition 3.3.8 below. See Theorem 5.3 of (CITE) for details, noting that Hoffman-Ohno use the extended map $\cdot : \mathfrak{h}^1 \otimes \mathfrak{h} \longrightarrow \mathfrak{h}$. I have restricted this to $\mathfrak{h}^1$ for simplicity, as I cannot see the purpose of the extension in future results.

3. One should check that this is well-defined, namely that the result is independent of how we decompose a word w into $w_1 w_2$, which can be done in many ways. This is insured by the co-associativity of Δ, which can easily be proved (c.f. [Hen]).

4. The last condition implies that

$$\begin{aligned} z_{a_1} \cdot 1 = z_{a_1} \cdot (1 \cdot 1) &= (1 \cdot 1)(z_{a_1} \cdot 1) + (z_{a_1} \cdot 1)(1 \cdot 1) \\ &= 2(z_{a_1} \cdot 1)\,, \end{aligned}$$

   since $\Delta(z_{a_1}) = 1 \otimes z_{a_1} + z_{a_1} \otimes 1$. This implies $z_{a_1} \cdot 1 = 0$, and by induction on length we can show that $u \cdot 1 = 0$ for all $1 \neq u \in \mathfrak{h}^1$.

Examples 3.3.5.

1. Take $u = z_3$ and $w = z_2 = xy$. Then $\Delta(u) = 1 \otimes z_3 + z_3 \otimes 1$, so
$$u \cdot w = (1 \cdot x)(z_3 \cdot y) + (z_3 \cdot x)(1 \cdot y) = xz_4 = z_5\,.$$
One can easily generalise this by induction to $z_n \cdot z_m = z_{n+m}$.

2. Take $u = z_3z_2$ and $w = z_2z_1$. We have $\Delta(u) = 1 \otimes z_3z_2 + z_3 \otimes z_2 + z_3z_2 \otimes 1$, so we obtain
$$\begin{aligned}
u \cdot w &= (1 \cdot z_2)(z_3z_2 \cdot z_1) + (z_3 \cdot z_2)(z_2 \cdot z_1) + (z_3z_2 \cdot z_2)(1 \cdot z_1)\\
&= (z_2)(0) + (z_3 \cdot xy)z_3 + (z_3z_2 \cdot xy)z_1\\
&= [(z_3 \cdot x)(1 \cdot y) + (1 \cdot x)(z_3 \cdot y)]\, z_3\\
&\quad + [(1 \cdot x)(z_3z_2 \cdot y) + (z_3 \cdot x)(z_2 \cdot y) + (z_3z_2 \cdot x)(1 \cdot y)]\, z_1\\
&= xz_4z_3\\
&= z_5z_3
\end{aligned}$$

As the example above suggests, computations can be cumbersome. The proposition below helps to make these a little more natural. It is stated in [HO] as being "immediate from the definitions", and we add our own short proof to make this clear.

Proposition 3.3.6. For all $w \in \mathfrak{h}^1$ we have $z_1 \cdot w = D(w)$, with D the standard derivation. Moreover, $z_n \cdot w = D_n(w)$ where D_n is the derivation satisfying $D(x) = 0$ and $D(y) = x^n y$.

Proof. By induction on the weight k of w. For $k = 0$, we have by the fourth remark above that $z_n \cdot 1 = 0 = D_n(1)$. For $k = 1$ we have from definitions that $z_n \cdot x = 0 = D_n(x)$, and $z_n \cdot y = z_{n+1} = x^n y = D_n(y)$. For weight $k \geq 2$, write $w = w_1w_2$ with w_1, w_2 of strictly lower weight. Then
$$\begin{aligned}
z_n \cdot w &= (1 \cdot w_1)(z_n \cdot w_2) + (z_n \cdot w_1)(1 \cdot w_2)\\
&= w_1(z_n \cdot w_2) + (z_n \cdot w_1)w_2\\
&= w_1D_n(w_2) + D_n(w_1)w_2\\
&= D_n(w)
\end{aligned}$$
which concludes the proof. □

The action of a letter z_n on a word w is now straightforward, but the action of a general word $u = z_{a_1} \dots z_{a_r}$ remains a little mysterious. The definition and proposition relate the action $\cdot$ to the stuffle product $*$, making it simpler and more intuitive.

Definition 3.3.7. For any sentence $a \in \mathfrak{h}^1$ and integer $r \geq 0$, define the 'length-filtering' map $L_r : \mathfrak{h}^1 \longrightarrow \mathfrak{h}^1$ as
$$L_r(a) = \sum_{w \in a,\, l(w)=r} w\,,$$
the sum of words in a of length r. Equivalently, L_r is the *linear* map such that
$$L_r(w) = \delta_{rl(w)}\, w$$
where δ_{ij} is the Kronecker delta.

Proposition 3.3.8. [HO, Lemma 5.2] For any words $u, w \in \mathfrak{h}^1$ with $l(w) = r$,

$$u \cdot w = L_r(u * w)\,.$$

Proof. In Appendix A.3. □

We are almost ready to state Ohno's relation. Let W_n the set of words in $\mathfrak{h}^1$ with weight n, and define the homogenous polynomial of weight n to be

$$h_n = \sum_{w \in W_n} w\,.$$

In other words, h_n is the sum of all words in $\mathfrak{h}^1$ of weight n, or the sum of all monomials in the z_i of weight n.

Example 3.3.9 (Inspired by Henderson)**.** Using the proposition above, the action $h_n \cdot w$ can be understood as the sum of all possible ways of increasing the weight of w by n while keeping its length intact. For $n = 3$ we have $h_3 = z_1^3 + z_1 z_2 + z_2 z_1 + z_3$, so taking a word $w = z_a$ gives

$$h_3 \cdot z_a = z_{a+3}$$

where most of the terms vanish. However, taking $w = z_a z_b$ gives

$$\begin{aligned} h_3 \cdot z_a z_b &= z_1^3 \cdot z_a z_b + z_1 z_2 \cdot z_a z_b + z_2 z_1 \cdot z_a z_b + z_3 \cdot z_a z_b \\ &= z_{a+1} z_{b+2} + z_{a+2} z_{b+1} + z_{a+3} z_b + z_a z_{b+3}\,, \end{aligned}$$

and we leave it as an easy exercise for the reader to see what happens for $w = z_a z_b z_c$ and beyond.

Inspired from this observation, we make the following proposition.

Proposition 3.3.10. For all words $w = z_{a_1} \dots z_{a_r} \in \mathfrak{h}^1$ and $n \geq 0$ we have

$$h_n \cdot w = \sum_{\substack{c_1 + \ldots + c_r = n \\ c_i \geq 0}} z_{a_1 + c_1} \dots z_{a_r + c_r}\,.$$

All we need to state Ohno's Theorem below is the action by h_n, so we really could have taken it to be defined by the equality in this proposition, as Ohno did in his original paper [Ohn]. However, the later exposition given in [HO] invokes the general action and states that the formulations are equivalent without proof. We give our own in Appendix A.3, which we did not find obvious. We are now ready to state the formulation of Ohno's Theorem presented [HO].

Theorem 3.3.11 (Ohno's Theorem)**.** For all words $w \in \mathfrak{h}^0$ and integer $n \geq 0$,

$$\zeta(h_n \cdot \tau(w)) = \zeta(h_n \cdot w)\,.$$

A direct proof can be found in [Ohn, Theorem 1], where it appears in the formulation of Proposition 3.3.10, which we have shown to be equivalent. To display the strength of Ohno's Theorem, we make explicit a few corollaries which we have already encountered before.

Firstly, the case $n = 0$ with $h_0 = 1$ specialises to the duality theorem

$$\zeta(\tau(w)) = \zeta(w)\,.$$

For $n = 1$ we have $h_1 = z_1$, so proposition 3.3.6 implies that $h_1 \cdot w = Dw$. Then Ohno's Theorem states that

$$\zeta(D\tau(w)) = \zeta(Dw)\,.$$

By the duality theorem we can take τ on the argument of the LHS to obtain Theorem 3.2.7

$$\zeta(\bar{D}w) = \zeta(Dw)\,,$$

or equivalently, Hoffman's relation

$$\zeta(w \,\text{ш}\, y - w * y) = 0\,.$$

Ohno's Theorem also implies the general sum formula given in Theorem 1.3.9, which was not proved up to now! Following [Ohn], take any $k \geq 3$ and $r > 0$ such that $k > r$. Let $w = z_{r+1} = x^r y$, implying that $\tau(w) = xy^r = z_2 z_1^{r-1}$. Taking $n = k - r - 1$, Proposition 3.3.10 gives

$$\zeta(h_n \cdot \tau(w)) = \sum_{\substack{c_1+\ldots+c_r=n \\ c_i \geq 0}} \zeta(2 + c_1, 1 + c_2 \ldots, 1 + c_r)\,, \qquad = \sum_{\substack{c_1+\ldots+c_r=k \\ c_1 \geq 2, c_i \geq 1}} \zeta(c_1, \ldots, c_r)\,,$$

whereas

$$\begin{aligned} \zeta(h_n \cdot w) &= \zeta(r + 1 + n) \\ &= \zeta(k)\,. \end{aligned}$$

By Ohno's Theorem, we obtain the general sum formula

$$\sum_{\substack{c_1+\ldots+c_r=n \\ c_1 \geq 2, c_i \geq 1}} \zeta(c_1, \ldots, c_r) = \zeta(k)$$

for any $k \geq 3$ and $k > r > 0$.

3.4 Derivation relations

In this section we state the derivation relations, a family which was proved to be equivalent to Ohno's Theorem in [IKZ].

For integer $n \geq 1$, define the derivation ∂_n such that

$$\partial_n(x) = x(x + y)^{n-1} y \qquad \text{and} \qquad \partial_n(y) = -x(x + y)^{n-1} y\,.$$

Theorem 3.4.1 (Derivation relations)**.** For all $w \in \mathfrak{h}^0$ and integer $n \geq 1$,

$$\zeta(\partial_n(w)) = 0\,.$$

Example 3.4.2. Taking $w = xy$ and $n = 3$ gives

$$\begin{aligned}\zeta(\partial_3(w)) &= \zeta(\partial_3(x)y + x\partial_3(y)) \\ &= \zeta(x(x+y)^2yy + xx(x+y)^2yy \\ &= \zeta(xyyyy + xyxyy - xxyxy - xxxxy) \\ &= \zeta(2,1,1,1) + \zeta(2,2,1) - \zeta(3,2) - \zeta(5)\,,\end{aligned}$$

which provides the derivation relation

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

Note that for $n = 1$ we have $\partial_1 = \bar{D} - D$, so the derivation relations also include Theorem 3.2.7 or equivalently, Hoffman's relation. Intriguingly, it is not clear how to obtain duality directly from the derivation relations, even though the equivalence theorem given further down guarantees that the relations it provides will be covered by *some* combination of derivation relations. In the same way, the EDS is expected to give all linear relations between MZVs, including those from (say) duality, but recovering them directly is out of reach for now.

We now state Theorem 3 of [IKZ], establishing the equivalence of Theorems 2.5.3 (EDS), 3.3.11 (Ohno) and 3.4.1 (derivation). This is a very impressing result which ties neatly together everything we have done so far. To be precise, the formulation we give below is less general and corresponds to the case $R = \mathbb{R}$, $Z_R = Z$.

Theorem 3.4.3 (Equivalence)**.** The following are equivalent.

1. $\zeta \circ f(w_0 ш w_1 - w_0 * w_1) = 0$ for all $w_0 \in \mathfrak{h}^0$ and $w_1 \in \mathfrak{h}^1$.
2. $\zeta(h_n \cdot \tau(w)) = \zeta(h_n \cdot w)$ for all $w \in \mathfrak{h}^0$ and integer $n \geq 0$.
3. $\zeta(\partial_n(w)) = 0$ for all $w \in \mathfrak{h}^0$ and integer $n \geq 1$.

Combining this with [IKZ, Th. 1,2] establishing the EDS as 1. above, the paper establishes all three claims at once. Not only this, but it gives us three alternative routes by which to attain each family of relations, the first being analytic while the others are algebraic in nature. Following the conjecture that the EDS generates everything, one can choose any one of three families above and hope to reach all possible relations among MZVs. This is a rather beautiful result and we encourage the reader to read the proof of equivalence in [IKZ], which is too long for the purpose of this report.

Another interesting difference between Ohno/derivations and the EDS is the following. Generating relations in weight k with the former involves choosing words w of weight k_1 and an integer n such that $k_1 + n = k$, where we think about increasing the weight of w by n. On the other hand, generating relations with the EDS involve choosing words w_0, w_1 of weights k_1, k_2 such that $k_1 + k_2 = k$, which can be though of as a 'convolution' or 'mixing' of words rather than the uniform increase of weight in one word.

Sections $1 - 3$ were aimed to introduce the reader to MZVs and tie together three seemingly different families of relations among them, which are expected to be equally powerful in producing all such relations. We have completed this objective and move on to a topic of a very different nature, namely interpolation. A characteristic feature of the rest of this report is that despite being inspired by other peoples' work as much as ever, a good majority is phrased in a different tone and perspective to that which one can find online. I have attempted to make it my own as much as possible, contributing small results while of course referencing inspiration and reproduction as always.

Chapter 4

Interpolation of MZVs

The first three sections follow Yamamoto's work in [Yam]. The fourth and beginning of fifth were inspired by Muneta's paper [Mun], but go far beyond. The sixth is our own.

4.1 Introduction: zeta star values

Upon generalising the Riemann zeta function at integer values to MZVs as

$$\zeta(a_1, \ldots, a_r) = \sum_{n_1 > \ldots > n_r > 0} \frac{1}{n_1^{a_1} \cdots n_r^{a_r}} \,,$$

a seemingly arbitrary choice was made as to whether we should take strict or non-strict inequalities for $n_1 > \ldots > n_r$. The alternative definition leads to the so-called (multiple) zeta *star* values (MZSV), considered early on by Hoffman but often discarded in preference of usual MZVs. The conditions for convergence are the same.

Definition 4.1.1. For any admissible multi-index $\mathbf{a} = (a_1, \ldots, a_r)$, define

$$\zeta^\star(\mathbf{a}) = \sum_{n_1 \geq \ldots \geq n_r > 0} \frac{1}{n_1^{a_1} \cdots n_r^{a_r}} \,.$$

Note that $\zeta^\star(k) = \zeta(k)$ for length 1, so this is indeed an alternative generalisation of the Riemann zeta values.

One can immediately notice that a zeta star value decomposes into a linear combination of MZVs, by splitting $n_i \geq n_j$ into the cases $n_i = n_j$ or $n_i > n_j$, somewhat similarly to the stuffle product. To make this precise, we follow Yamamoto in [Yam] by letting P the set of multi-indices

$$P = \{(a_1 \square \ldots \square a_n) \mid \square \in \{, , +\}\}$$

in which each $\square$ is either a comma , or a plus $+$. We should really write P as $P_{\mathbf{a}}$, but we will omit this whenever the context is clear. Then we obtain

$$\zeta^\star(\mathbf{a}) = \sum_{\mathbf{p} \in P} \zeta(\mathbf{p}) \,. \tag{†}$$

Example 4.1.2. Taking $\mathbf{a} = (4,2,3)$ gives

$$\begin{aligned}
\zeta^\star(4,2,3) &= \sum_{n_1 \geq n_2 \geq n_3 > 0} \frac{1}{n_1^4 n_2^2 n_3^3} \\
&= \Big(\sum_{n_1 > n_2 \geq n_3 > 0} + \sum_{n_1 = n_2 \geq n_3 > 0} \Big) \frac{1}{n_1^4 n_2^2 n_3^3} \\
&= \Big(\sum_{n_1 > n_2 > n_3 > 0} + \sum_{n_1 > n_2 = n_3 > 0} + \sum_{n_1 = n_2 \geq n_3 > 0} + \sum_{n_1 = n_2 = n_3 > 0} \Big) \frac{1}{n_1^4 n_2^2 n_3^3} \\
&= \zeta(4,2,3) + \sum_{n_1 > n_2 = n_3 > 0} \frac{1}{n_1^4 n_2^{2+3}} + \sum_{n_1 = n_2 \geq n_3 > 0} \frac{1}{n_1^{4+2} n_3^3} + \sum_{n_1 = n_2 = n_3 > 0} \frac{1}{n_1^{4+2+3}} \\
&= \zeta(4,2,3) + \zeta(4,5) + \zeta(6,3) + \zeta(9)\,.
\end{aligned}$$

The formula (†) expresses star-zetas as a linear combination of zetas, and we will later see how to perform the converse, i.e. writing zetas in terms of star-zetas. Moreover, there are counterparts to many relations that we have seen among MZVs, among them the sum formula analogue:

$$\sum_{\substack{r_1 + \ldots + r_n = k \\ r_1 \geq 2,\ r_i \geq 1}} \zeta^\star(r_1, \ldots, r_n) = \binom{k-1}{n-1} \zeta^\star(k)\,.$$

We will also see that the double shuffle extends to zeta star values, and so does the EDS. We give a quick preview of how formulae for stuffle and shuffle products may change accordingly. Recall that to express the product of MZVs, we defined a map $Z : \mathfrak{h}^0 \longrightarrow \mathbb{R}$ such that

$$\begin{aligned}
Z(z_{a_1} \ldots z_{a_r}) &= \zeta(a_1, \ldots, a_r) \\
Z(u * v) &= Z(u) Z(v)\,,
\end{aligned}$$

where the stuffle product was given by

$$z_i u * z_j v = z_i(u * z_j v) + z_j(z_i u * v) + z_{i+j}(u * v)\,.$$

For MZSVs, the same formula does not hold. We want to define a similar map $Z^\star : \mathfrak{h}^0 \longrightarrow \mathbb{R}$ such that

$$\begin{aligned}
Z^\star(z_{a_1} \ldots z_{a_r}) &= \zeta(a_1, \ldots, a_r) \\
Z^\star(u \star v) &= Z^\star(u) Z^\star(v)\,,
\end{aligned}$$

for some product $\star$, but taking $\star = *$ as above does not work. Instead we must define a slightly different stuffle product given by

$$z_n u \star z_m v = z_n(u \star z_m v) + z_m(z_n u \star v) - z_{n+m}(u \star v)\,,$$

which will give us the required statement $Z^\star(u \star v) = Z^\star(u) Z^\star(v)$. The proof that this formula works will come in the next section. The point of this is to illustrate the structural difference between MZVs and MZSVs, giving us a hint as to why we may look into one rather than the other, depending on how 'nice' their algebraic properties are.

Instead of the binary viewpoint of zeta vs zeta-star, one might ask whether there is a continuous deformation from one to the other. Yamamoto's definition of t-zeta values accomplishes exactly this, which we expose and build on in this chapter. It will turn out that the 'midpoint' or 'halfway' of this deformation exhibits an elegant property, to which we come in section 3.

4.2 Interpolation

In this section we follow Yamamoto's paper [Yam], adding to his explanations and proofs.

Given a multi-index $\mathbf{p} = (a_1 \square \ldots \square a_r) \in P_{\mathbf{a}}$, define $\sigma(\mathbf{p})$ to be the number of $+$ used in $\mathbf{p}$,

$$\sigma(\mathbf{p}) = \#\{\square \text{ in } \mathbf{p} \mid \square = +\}\,.$$

Equivalently, note that

$$\sigma(\mathbf{p}) = r - \#\{\text{commas in } \mathbf{p}\} = l(\mathbf{a}) - l(\mathbf{p})\,.$$

Definition 4.2.1. For any admissible multi-index $\mathbf{a}$, define

$$\zeta^t(\mathbf{a}) = \sum_{\mathbf{p} \in P} t^{\sigma(\mathbf{p})} \zeta(\mathbf{p})\,.$$

This polynomial in one variable t was introduced by Yamamoto as a way to 'interpolate' (or deform) between zeta and zeta-star. Indeed, notice that

$$\zeta^0(\mathbf{a}) = \zeta(\mathbf{a}) \qquad \text{and} \qquad \zeta^1(\mathbf{a}) = \zeta^\star(\mathbf{a})\,.$$

The first equality comes from $0^0 = 1$ for $\sigma(\mathbf{p}) = 0 \iff \mathbf{p} = \mathbf{a}$, and the second from equation (†). By virtue of being a polynomial, the deformation is continuous in t. We will call $\zeta^t(\mathbf{a})$ a t-zeta value or t-zeta for admissible $\mathbf{a}$.

Remark 4.2.2. Note that t is a formal variable, but we can view it (and evaluate it) as lying in $\mathbb{R}$, which will be useful later on. We have also thought of complexifying t, perhaps giving complex t-zetas which are structurally elegant. This can be performed without affecting any of the previous discussion, so that $t \in \mathbb{R}$ can be replaced everywhere with $t \in \mathbb{C}$. We have not found a particular value of t for which this has unique applications, although it may broaden the scope of future possibilities.

Example 4.2.3. Take $\mathbf{a} = (3, 2, 1)$. Then

$$\zeta^t(3,2,1) = \zeta(3,2,1) + t\zeta(5,1) + t\zeta(3,3) + t^2\zeta(6)\,,$$

which specialises to

$$\begin{aligned}
&\zeta^0(3,2,1) = \zeta(3,2,1)\\
&\zeta^1(3,2,1) = \zeta^\star(3,2,1) = \zeta(3,2,1) + \zeta(5,1) + \zeta(3,3) + \zeta(6)\,.
\end{aligned}$$

In order to take the product of t-zetas, we need to make this interpolation more formal. To do so, we extend the map $Z = \zeta : \mathfrak{h}^0 \longrightarrow \mathbb{R}$ to $\mathfrak{h}^0[t]$ linearly, using the same letter Z.

Definition 4.2.4. Define the $\mathbb{Q}[t]$-linear map $Z : \mathfrak{h}^0[t] \longrightarrow \mathbb{R}[t]$ by

$$Z(z_{a_1} \dots z_{a_r}) = \zeta(a_1, \dots, a_r)\,.$$

We will often denote Z by ζ. We now introduce Yamamoto's interpolating operator S^t.

Definition 4.2.5. Define the $\mathbb{Q}[t]$-linear map $S^t : \mathfrak{h}^1[t] \longrightarrow \mathfrak{h}^1[t]$ as

$$S^t(1) = 1, \qquad S^t(z_a w) = z_a S^t(w) + t z_a \circ S^t(w)\,.$$

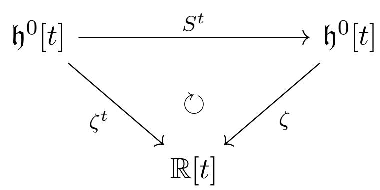
for letters $z_a \in \mathcal{A}$ and words $w \in \mathfrak{h}^1$.

It is immediate to see that S^t respects weight. The interpolating operator is constructed to reflect our definition of t-zetas, as the following proposition makes explicit. For the statement to make sense, we leave it as an easy exercise to the reader to show that $S^t(\mathfrak{h}^0[t]) \subset \mathfrak{h}^0[t]$, and moreover notice that S^t respects weight.

Proposition 4.2.6. Let $Z^t = Z \circ S^t : \mathfrak{h}^0[t] \longrightarrow \mathbb{R}[t]$. Then

$$Z^t(z_{a_1} \dots z_{a_r}) = \zeta^t(a_1, \dots, a_r)\,.$$

In other words, given $w \in \mathfrak{h}^0$ corresponding to an MZV $\zeta(\mathbf{a})$, the sentence $S^t(w)$ corresponds to the MZV $\zeta^t(\mathbf{a})$ by our usual identification through $Z = \zeta$. This is why we call S^t the interpolating operator, allowing us to shift from usual zetas to t-zetas with ease. The following commutative diagram illustrates this fact, abusing notation $Z^t = \zeta^t$ as usual.



Proof. In Appendix A.4 □

Remark 4.2.7. Recall that $\zeta^0(\mathbf{a}) = \zeta(\mathbf{a})$ and $\zeta^1(\mathbf{a}) = \zeta^\star(\mathbf{a})$. Mirroring these equalities, notice that S^0 is the identity map while S^1 takes MZVs to MZSVs, in the sense that

$$Z^1(z_{a_1} \dots z_{a_r}) = \zeta^1(a_1, \dots, a_r) = \zeta^\star(a_1, \dots, a_r)\,,$$

which corresponds to the map $Z^\star$ we wanted to define in section 4.1. In other words, $Z^0 = Z$ and $Z^1 = Z^\star$.

Before moving on to the product of t-zetas, we state a result which we have discovered alone. This proposition is essentially an application of duality to t-zetas at $t = -1$.

Proposition 4.2.8. For any odd $n \geq 1$,

$$\zeta^{-1}(2, \{1\}^n) = 0\,.$$

Proof. In Appendix A.4. □

4.3 The t-stuffle product

In the first section, it was foreshadowed that we could construct a stuffle product $\star$ so as to obtain

$$Z^\star(u \star v) = Z^\star(u)Z^\star(v)\,.$$

In this section we give Yamamoto's general t-stuffle product $\overset{t}{*}\colon \mathfrak{h}^1[t] \longrightarrow \mathfrak{h}^1[t]$ which will satisfy

$$Z^t(u \overset{t}{*} v) = Z^t(u)Z^t(v)$$

for all $u, v \in \mathfrak{h}^0[t]$. This product will specialise to $*$ and $\star$ for $t = 0$ and $t = 1$ respectively, giving us the desired result and much more.

First, we use the circle product to define the action $\circ$ of $\mathcal{A}$ on $\mathfrak{h}^1[t]$ by

$$z_n \circ 1 = 0 \qquad \text{and} \qquad z_n \circ (z_m w) = (z_n \circ z_m)w$$

for words $w \in \mathfrak{h}^1[t]$, extended $\mathbb{Q}[t]$-linearly.

Definition 4.3.1. The t-stuffle product $\overset{t}{*}$ on $\mathfrak{h}^1[t]$ is defined recursively by:

$$\begin{aligned} 1 \overset{t}{*} u = u \overset{t}{*} 1 &= u \\ au \overset{t}{*} bv &= a(u \overset{t}{*} bv) + b(au \overset{t}{*} v) + (1-2t)(a \circ b)(u \overset{t}{*} v) \\ &\quad + (t^2 - t)(a \circ b) \circ (u \overset{t}{*} v) \end{aligned}$$

for all letters $a, b \in \mathcal{A}$ and words $u, v \in \mathfrak{h}^1[t]$, extended $\mathbb{Q}[t]$-linearly.

Remark 4.3.2. We have $\overset{0}{*} = *$ as expected, and $\overset{1}{*} = \star$ as pre-emptively defined in the first section by

$$z_n u \star z_m v = z_n(u \star z_m v) + z_m(z_n u \star v) - (z_n \circ z_m)(u \star v)\,.$$

Moreover, the t-stuffle product is associative, commutative and respects weight, which will be shown near the end of this section, in Remark 4.3.7.

Example 4.3.3. Take $u = z_2 z_2$ and $v = z_3$. Then

$$\begin{aligned} u \overset{t}{*} v &= z_2(z_2 \overset{t}{*} z_3) + z_3(z_2 z_2 \overset{t}{*} 1) + (1-2t)(z_2 \circ z_3)(z_2 \overset{t}{*} 1) + (t^2 - t)(z_2 \circ z_3) \circ (z_2 \overset{t}{*} 1) \\ &= z_2\left[z_2 z_3 + z_3 z_2 + (1-2t)z_5 + (t^2 - t)\cdot 0\right] + z_3 z_2 z_2 + (1-2t)z_5 z_2 + (t^2-t)z_7 \\ &= z_2 z_2 z_3 + z_2 z_3 z_2 + z_3 z_2 z_2 + (1-2t)(z_2 z_5 + z_5 z_2) + (t^2 - t)z_7\,. \end{aligned}$$

For $t = 0$ and $t = 1$, this specialises to the usual shuffle and star-shuffle products:

$$\begin{aligned} u * v &= z_2 z_2 z_3 + z_2 z_3 z_2 + z_3 z_2 z_2 + z_2 z_5 + z_5 z_2 \\ u \star v &= z_2 z_2 z_3 + z_2 z_3 z_2 + z_3 z_2 z_2 - z_2 z_5 - z_5 z_2\,. \end{aligned}$$

The aim of this section is to prove the following theorem.

Theorem 4.3.4. The map $Z^t : (\mathfrak{h}^0[t], \overset{t}{*}) \longrightarrow (\mathbb{R}[t], \cdot)$ is a $\mathbb{Q}[t]$-algebra homomorphism.

In the example above, this would imply

$$\zeta^t(2,2)\zeta^t(3) = \zeta^t(2,2,3) + \zeta^t(2,3,2) + \zeta^t(3,2,2) + (1-2t)(\zeta^t(2,5) + \zeta^t(5,2)) + (t^2 - t)\zeta^t(7)\,.$$

To establish the theorem, we do *not* need to follow a similar proof as for MZV stuffle and shuffle products, which would be messy. Instead, we use the crucial fact that $Z^t = Z \circ S^t$ to transfer the problem to that of the stuffle. We already know that $Z : (\mathfrak{h}^0[t], *) \longrightarrow (\mathbb{R}, \cdot)$ is a homomorphism by $\mathbb{Q}[t]$-linear extension of Theorem 2.2.14, so it remains only to prove the following.

Theorem 4.3.5. The map $S^t : (\mathfrak{h}^1[t], \overset{t}{*}) \longrightarrow (\mathfrak{h}^1[t], *)$ is a homomorphism.

This implies Theorem 4.3.4 because a composition of morphisms is a morphism. More precisely,

$$Z^t(u \overset{t}{*} v) := Z(S^t(u \overset{t}{*} v)) = Z(S^t(u) * S^t(v)) = Z(S^t(u))Z(S^t(v)) = Z^t(u)Z^t(v)\,,$$

so that Z^t is a homomorphism.

The proof of Theorem 4.3.5 can be found in [Yam, Theorem 3.6], but I reproduce it individually in the context of finding both stuffle and shuffle products for t-zetas in the next sections. Our proof is very similar to Yamamoto's, but we work through it in Appendix A.4 with variations in style and more detail.

We begin by a simple but crucial lemma, the first three equalities of which were introduced in [IKOO, Lemmata 1,2] and the fourth is our own. The motivation for its necessity is the following problem: we have a formula to take the stuffle product of two elements au and bv. However, the operator S^t will give rise to elements of the type $a \circ u$, which we will need to stuffle with elements of the type bv or $b \circ v$. How can we do this, or at least how can we rewrite the stuffle in a useful way?

Lemma 4.3.6. For any letters $a, b \in \mathcal{A}$ and words $u, v \in \mathfrak{h}^1$, the following equalities hold.

$$(a \circ u) * (bv) = a \circ (u * bv) + b((a \circ u) * v) - (a \circ b)(u * v) \tag{1}$$
$$(au) * (b \circ v) = b \circ (au * v) + a(u * (b \circ v)) - (a \circ b)(u * v) \tag{2}$$
$$(a \circ u) * (b \circ v) = a \circ (u * (b \circ v)) + b \circ ((a \circ u) * v) - (a \circ b) \circ (u * v) \tag{3}$$
$$S^t(a \circ u) = a \circ S^t(u)\,. \tag{4}$$

Both this lemma and Theorem 4.3.5 are proved in Appendix A.4.

Remark 4.3.7. S^t is in fact an isomorphism, with inverse S^{-t}. Note that S^t is defined for all $t \in \mathbb{R}$, and we have $S^t \circ S^{-t}(1) = S^t(1) = 1$. Then by induction on word length,

$$\begin{aligned} S^t \circ S^{-t}(aw) &= S^t(aS^{-t}(w) - ta \circ S^{-t}(w)) \\ &= aS^t(S^{-t}(w)) + ta \circ S^t(S^{-t}(w)) - ta \circ S^t(S^{-t}(w)) \\ &= aw + ta \circ w - ta \circ w \\ &= aw\,, \end{aligned}$$

from which we conclude that $S^t \circ S^{-t} = I$ is the identity map. The third term of the second equality follows from equation (4) above.

This isomorphism is powerful and will be used throughout, in particular to prove the following two propositions.

Proposition 4.3.8. We can invert the definition

$$\zeta^t(\mathbf{a}) = \sum_{\mathbf{p}\in P} t^{\sigma(\mathbf{p})}\zeta(\mathbf{p})$$

by the formula

$$\zeta(\mathbf{a}) = \sum_{\mathbf{p}\in P} (-t)^{\sigma(\mathbf{p})}\zeta^t(\mathbf{p})\,.$$

Proof. This is immediate from the inverse of S^t being S^{-t}. More precisely, write $\bar{\mathbf{a}} = u \in \mathfrak{h}^0$ and recall from the proof of Proposition 4.2.6 that

$$S^t(u) = \sum_{w\in W} t^{\sigma(w)} w\,,$$

where W corresponds to P and w corresponds to $\mathbf{p}$. Then we obtain

$$\begin{aligned}\zeta(\mathbf{a}) &= Z(u) = Z(S^t \circ S^{-t}(u)) = Z^t(S^{-t}(u)) \\ &= \sum_{w\in W} (-t)^{\sigma(w)} Z^t(w) = \sum_{\mathbf{p}\in P} (-t)^{\sigma(\mathbf{p})}\zeta^t(\mathbf{p})\,.\end{aligned}$$ □

Proposition 4.3.9. The t-stuffle is associative, commutative and respects weight.

Proof. In Appendix A.4. □

The t-stuffle formula can appear to be plucked out of thin air, but the process of finding it involves essentially a reverse process of the proof given above. One is then *forced* to choose the product like this, and there is no other way of defining appropriately. The essential reason is that S^t is invertible, but I will not go into explaining the details of this.

We now explain the first reason for having taken an interest in t-zetas at all. Yamamoto applies the case $t = 1/2$ to the *two-one formula* conjectured in [OZ]. We quickly review this application at the end of this section but begin with a different direction which we have found independently, although it was no doubt noticed by him.

Looking at the formula for the t-stuffle

$$au \overset{t}{*} bv = a(u \overset{t}{*} bv) + b(au \overset{t}{*} v) + (1-2t)(a \circ b)(u \overset{t}{*} v) + (t^2 - t)(a\circ b)\circ(u \overset{t}{*} v)\,,$$

we see that the fourth term is eliminated for both $t = 0$ and $t = 1$, which correspond to MZVs and MZSVs respectively, suggesting that they have 'nicer' (simpler) structure when taking products. However, we could also try to eliminate the third term, leading to $t = 1/2$ and the formula

$$au \overset{1/2}{*} bv = a(u \overset{t}{*} bv) + b(au \overset{1/2}{*} v) - \frac{1}{4}(a\circ b)\circ(u \overset{1/2}{*} v)\,.$$

This is the only other t-zeta which has only three terms in its stuffle product, and suggests that it may be worth investigating in particular. Indeed, half-zetas have the following property.

Proposition 4.3.10. Take any words $u, v \in \mathfrak{h}^1$ of length r, s. Then all words in $u \overset{1/2}{*} v$ have length in the set

$$\{r+s,\ r+s-2,\ \ldots\} = \{1 \le n \le r+s \mid n \equiv r+s \mod 2\}\,.$$

In other words, if $r+s$ is even (resp. odd) then all words have even (resp. odd) length.

This has the interesting corollary that the product of half-zetas 'jumps' length, in the sense that only zetas of even or odd lengths appear.

Proof. Looking at the half-stuffle formula should give the reader an immediate idea as to why this is true. The first two terms

$$a(u \overset{t}{*} bv) + b(au \overset{1/2}{*} v)$$

of the stuffle formula do not alter the length since concatenation is used on the left-hand side. The third term

$$(a \circ b) \circ (u \overset{1/2}{*} v)$$

reduces the length by 1 upon taking $a \circ b$, and once more when taking $\circ$ with $u \overset{1/2}{*} v$. Altogether the length decreases by 0 or 2, conserving parity at each recursive step and therefore overall. □

Example 4.3.11. Take $u = z_2$ and $v = z_2$. Then

$$u \overset{1/2}{*} v = z_2 z_2 + z_2 z_2 - \frac{1}{4}(z_2 \circ z_2) \circ (1) = 2 z_2 z_2\,.$$

Using Theorem 4.3.4, this implies

$$\zeta^{\frac{1}{2}}(2)\zeta^{\frac{1}{2}}(2) = 2\zeta^{\frac{1}{2}}(2,2)\,,$$

which is a more elegant formula than the MZV equivalent:

$$\zeta(2)\zeta(2) = 2\zeta(2,2) + \zeta(4)\,,$$

where the term $\zeta(4)$ comes from the third term of the stuffle product, which is not present for half-zetas! A useful exercise to see 'why' this is true (beyond our results saying so!) is to use the definition of t-zetas. At $t = 1/2$, we have $\zeta^{\frac{1}{2}}(2) = \zeta(2)$ and $\zeta^{\frac{1}{2}}(2,2) = \zeta(2,2) + \frac{1}{2}\zeta(4)$. It follows that

$$\zeta^{\frac{1}{2}}(2)\zeta^{\frac{1}{2}}(2) = \zeta(2)\zeta(2) = 2\zeta(2,2) + \zeta(4) = 2(\zeta(2,2) + \frac{1}{2}\zeta(4)) = 2\zeta^{\frac{1}{2}}(2,2)\,.$$

In this example, we have translated the problem of finding the product of half-zetas by writing them as zetas, taking the usual stuffle product, and then re-expressing the result in terms of half-zetas. This mirrors the idea of using the interpolating operator as a way of making the t-stuffle descend into the usual stuffle.

Example 4.3.12. My supervisor invited me to look at some relations written in his 'research blog', which seemed to exhibit some length-preserving structure that wasn't well-understood or accounted for. One of them is the following, which I have checked numerically to high numerical precision:

$$\begin{aligned}15\zeta(7,5,3)+6\zeta(5,7,3)+36\zeta(5,5,5)-14\zeta(9,3,3)\\ +\frac{15}{2}\zeta(7,8)+18\zeta(10,5)+\frac{7}{2}\zeta(12,3)+21\zeta(5,10)-7\zeta(9,6)=\frac{17}{20}\zeta(15)\,.\end{aligned}$$

One can immediately notice some striking properties of the relation's coefficients. In particular, the coefficients of $\zeta(9,6)$, $\zeta(7,8)$ and $\zeta(10,5)$ are half those of $\zeta(9,3,3)$, $\zeta(7,5,3)$ and $\zeta(5,5,5)$, with indices of the former being sums of the latter. The other coefficients are also related in this way. As such, we can write the relation with half-zetas in the immensely more elegant form of:

$$15\zeta^{\frac{1}{2}}(7,5,3)+6\zeta^{\frac{1}{2}}(5,7,3)+36\zeta^{\frac{1}{2}}(5,5,5)-14\zeta^{\frac{1}{2}}(9,3,3)=\frac{58}{5}\zeta^{\frac{1}{2}}(15)\,. \tag{††}$$

Notice that this relation 'skips' length, as there are no even-length zetas involved in the relation. From our previous considerations, this suggests that it comes from the stuffle product in some way. Although we do not make this explicit in full detail, it does indeed arise from a product. Instead of comparing stuffle and shuffle, the idea is to take an existing relation in lower weight and take the product of the relation with another MZV, which will preserve length through the stuffle. This is a powerful bridge between relations of different weight, which *a priori* may not exist, and can induce relations by induction on the weight.

In our case, we use the relation found by [GKZ, p. 2] in weight 12, originating in an interesting way through cusp forms (this justifies the presence of the mysterious 691 coefficient, which appears in the 12th Eisenstein series):

$$28\zeta(9,3)+150\zeta(7,5)+168\zeta(5,7)=\frac{5197}{691}\zeta(12)\,.$$

This can be rewritten for half-zetas as

$$28\zeta^{\frac{1}{2}}(9,3)+150\zeta^{\frac{1}{2}}(7,5)+168\zeta^{\frac{1}{2}}(5,7)=\frac{124740}{691}\zeta(12)\,.$$

Now take the product of both sides with $\zeta^{\frac{1}{2}}(3)$, and expand using the half-stuffle product. This gives

$$\begin{aligned}28\left[2\zeta^{\frac{1}{2}}(9,3,3)-\frac{1}{4}\zeta^{\frac{1}{2}}(15)\right]+150\left[\zeta^{\frac{1}{2}}(7,5,3)+\zeta^{\frac{1}{2}}(7,3,5)+\zeta^{\frac{1}{2}}(3,7,5)-\frac{1}{4}\zeta^{\frac{1}{2}}(15)\right]+\\ 168\left[\zeta^{\frac{1}{2}}(5,7,3)+\zeta^{\frac{1}{2}}(5,3,7)+\zeta^{\frac{1}{2}}(3,5,7)-\frac{1}{4}\zeta^{\frac{1}{2}}(15)\right]=\frac{124740}{691}\left[\zeta^{\frac{1}{2}}(12,3)+\zeta^{\frac{1}{2}}(3,12)\right]\,.\end{aligned}$$

Now the LHS involves most of the terms which appear in (††), and are only of length 3 or 1 thanks to the half-stuffle. The extra terms, which are unwanted, can be removed by using other relations in lower weight. The RHS is slightly more delicate, involving terms of length 2. One remedy is to find a second relation expressing $\zeta^{\frac{1}{2}}(12)$ in terms of length 2 zetas only, for which the stuffle will give required length. For instance, we can use the t-zeta analogue of Euler's sum theorem given in Section 4.5. Note that the process described above is inductive: assuming we re-express $\zeta^{\frac{1}{2}}(12)$ appropriately, we have found a relation in low weight (12) of uniform length-parity (2). Taking the half-stuffle product with some other half-zeta, this gives another relation in higher weight (15) which is also uniform in length-parity (1 and 3)!

Remark 4.3.13. It may sometimes be useful to work 'modulo products' to study MZVs, at which point the half-stuffle is even more powerful. Indeed, the product will be put to 0 whereas its half-stuffle expansion will be uniform in length-parity, which gives a relation among half-zetas of same length-parity *modulo products*.

Finally, we give another algebraic property unique to half-zetas and an application related to the two-one formula, following [Yam, Chap. 4]. First define $y_j = 2z_{2j+1}$ for $j = 0, 1, 2, \dots$ and let $\mathfrak{h}^{0,odd} \subset \mathfrak{h}^0$ the subalgebra of $\mathfrak{h}^0$ generated by the letters y_j. The idea is that taking the half-stuffle product of two elements in this subalgebra remains in this subalgebra, because each step of the half-stuffle either concatenates these letters or adds the values of three of them together, but the sum of three odd numbers is odd. The following proposition, from [Yam, Prop. 4.3], makes this precise. Note also that Yamamoto's statement contains a mistake which I have corrected.

Proposition 4.3.14. $(\mathfrak{h}^{0,odd}, \overset{1/2}{*})$ is a subalgebra of $(\mathfrak{h}^0, \overset{1/2}{*})$. More precisely,

$$y_i w \overset{1/2}{*} y_j w' = y_i(w \overset{1/2}{*} w') + y_j(y_i w \overset{1/2}{*} w') - z_{2(i+j+1)} \circ (w \overset{1/2}{*} w') \,.$$

Moreover, the linear map $Z_{\text{odd}} : (\mathfrak{h}^{0,odd}, \overset{1/2}{*}) \longrightarrow (\mathbb{R}, \cdot)$ given by

$$Z_{\text{odd}}(y_{j_1} \dots y_{j_n}) = 2^n \zeta^{\frac{1}{2}}(2j_1 + 1, \dots, 2j_n + 1)$$

is an algebra homomorphism.

Proof. The first two terms of the stuffle product involve only letters y_i. By induction on length, assume that all words u in $w \overset{1/2}{*} w'$ begin with some letter y_k. Then the third term of the product is

$$-z_{2(i+j+1)} \circ y_i u = -2z_{2(i+j+k+1)+1} u = -2y_{i+j+k+1} u \,,$$

which also begins with such a letter. It follows that $(\mathfrak{h}^{0,odd}, \overset{1/2}{*})$ is a subalgebra with respect to the half-stuffle. The second claim holds immediately from Theorem 4.3.4, which provides an algebra homomorphism for any given subalgebra. □

To conclude this section, we give an application relating to the two-one formula, conjectured in [OZ] and recently proved by Zhao (as yet unpublished).

Theorem 4.3.15 (Two-one formula)**.** For integers $n, j_1 \geq 1$ and $j_2, \dots, j_n \geq 0$,

$$\zeta^\star(\{2\}^{j_1}, 1, \dots, \{2\}^{j_n}, 1) = 2^n \zeta^{\frac{1}{2}}(2j_1 + 1, \dots, 2j_n + 1) \,.$$

Together with Proposition 4.3.14, the two-one formula immediately implies the following result.

Corollary 4.3.16. The linear map $X : (\mathfrak{h}^{0,odd}, \overset{1/2}{*}) \longrightarrow (\mathbb{R}, \cdot)$ defined by

$$X(y_{j_1} \dots y_{j_n}) = \zeta^\star(\{2\}^{j_1}, 1, \dots, \{2\}^{j_n}, 1)$$

is an algebra homomorphism.

Having provided examples of the usefulness of t-zetas (particularly half-zetas), we proceed to the t-shuffle product and further analogues of the tools involved in studying usual MZVs.

4.4 The t-shuffle product

Inspired from Yamamoto's t-stuffle product, we define a t-shuffle product which mirrors the product of t-zetas as usual. This will lead us to generalising the double shuffle relation to t-zetas, and the next section will show that we can extend it as for usual zetas. Finding the t-shuffle product was my own initiative and work, but much of my results were propelled by Muneta's construction of a shuffle product for star-zetas in [Mun], which we generalise to t-zetas.

Before we proceed, define

$$\delta(w) = \begin{cases} 1 & \text{if } w = 1 \\ 0 & \text{otherwise} \end{cases}$$

for all words $w \in \mathfrak{h}^1$, which we extend $\mathbb{Q}[t]$-linearly to sentences in $\mathfrak{h}^1[t]$.

Definition 4.4.1. The t-shuffle product $\overset{t}{ш}$ on $\mathfrak{h}^1[t]$ is defined recursively by:

$$\begin{aligned} 1 \overset{t}{ш} u &= u \overset{t}{ш} 1 = u \\ au \overset{t}{ш} bv &= a(u \overset{t}{ш} bv) + b(au \overset{t}{ш} v) - t\delta(u)xbv - t\delta(v)xau \end{aligned}$$

for all letters $a, b \in A$ and words $u, v \in \mathfrak{h}^1[t]$, extended $\mathbb{Q}[t]$-linearly.

Remark 4.4.2. As was proved for the t-stuffle, the t-shuffle is associative, commutative and respects weight. Unlike the t-stuffle, it is moreover linear in t.

Example 4.4.3. Taking $w = xy$ and $w' = xy$ and using commutativity of the t-shuffle,

$$\begin{aligned} w \overset{t}{ш} w' &= x(y \overset{t}{ш} xy) + x(xy \overset{t}{ш} y) - 0 - 0 \\ &= 2x[yxy + x(y \overset{t}{ш} y) - txxy - 0] \\ &= 2x[yxy + x(2yy - 2txy) - txxy] \\ &= 2xyxy + 4xxyy - 6txxxy\,. \end{aligned}$$

Again, the main aim of this section is to prove the following.

Theorem 4.4.4. The map $Z^t : (\mathfrak{h}^0[t], \overset{t}{ш}) \longrightarrow (\mathbb{R}[t], \cdot)$ is a $\mathbb{Q}[t]$-algebra homomorphism.

In the example above, this would imply

$$\zeta^t(2)\zeta^t(2) = 2\zeta^t(2,2) + 4\zeta^t(3,1) - 6t\zeta^t(4)\,,$$

which specialises at $t = 0$ to the known

$$\zeta(2)\zeta(2) = 2\zeta(2,2) + 4\zeta(3,1)$$

and at $t = 1$ to the new, non-trivial relation

$$\zeta^\star(2)\zeta^\star(2) = 2\zeta^\star(2,2) + 4\zeta^\star(3,1) - 6\zeta^\star(4)\,.$$

Remark 4.4.5. There is a good reason for which the numbers above satisfy $2+4=6$. Using definition, we have $\zeta^\star(2)=\zeta(2)$, $\zeta^\star(2,2)=\zeta(2,2)+\zeta(4)$ and $\zeta^\star(3,1)=\zeta(2,2)+\zeta(4)$. By the known shuffle product, this implies

$$\begin{aligned}\zeta^\star(2)\zeta^\star(2)=\zeta(2)\zeta(2)=2\zeta(2,2)+4\zeta(3,1)&=2(\zeta(2,2)+\zeta(4))+4(\zeta(3,1)+\zeta(4))-6\zeta(4)\\ &=2\zeta^\star(2,2)+4\zeta^\star(3,1)-6\zeta^\star(4)\,!\end{aligned}$$

We now proceed as for the t-stuffle, noting that $Z:(\mathfrak{h}^0[t],*)\longrightarrow(\mathbb{R},\cdot)$ is a homomorphism by $\mathbb{Q}[t]$-linear extension of Theorem 2.3.11. It remains only to prove the following.

Theorem 4.4.6. The map $S^t:(\mathfrak{h}^1[t],\overset{t}{ш})\longrightarrow(\mathfrak{h}^1[t],ш)$ is a homomorphism.

Before proving this claim, we must notice that our definition of S^t hinges on letters $z\in\mathcal{A}$ and their circle product. This does not fit well with the t-shuffle product, which is defined through letters $x,y\in A$. As a result, we must find an alternative definition of S^t on such letters.

Definition 4.4.7. Define the linear map $R^t:\mathfrak{h}^1[t]\longrightarrow\mathfrak{h}^1[t]$ as

$$R^t(1)=1,\qquad R^t(x)=x,\qquad R^t(y)=y+tx,\qquad R^t(uv)=R^t(u)R^t(v)$$

for all words $u,v\in\mathfrak{h}^1$.

In Muneta's work, this map is called S_1, which we rename both for notational ease and to emphasise the presence of the variable t, which Muneta does not invoke since he is only looking at MZSVs and MZVs, not their interpolation.

Proposition 4.4.8. For any word $w=uy\in\mathfrak{h}^1[t]$, the map S^t satisfies

$$S^t(uy)=R^t(u)y\,.$$

Note that this brings to life an alternative definition of S^t on letters x,y, *except for* its action on the word 1, which cannot be written as uy. This will be linked to the two last terms of the t-shuffle product, which can be viewed as 'exceptions' coming from the last step of the recursive process, where at least one of the words is 1.

Proof. In Appendix A.4, by a standard induction on length. □

Remark 4.4.9. The proposition above implies that for any words $u,v\in\mathfrak{h}^1[t]$ with $v\neq1$, we have

$$S^t(uv)=R^t(u)S^t(v)\,.$$

This will be crucial in the proof of Theorem 4.4.6, which is given in Appendix A.4 and implies our main Theorem 4.4.4.

As for the t-stuffle, what values of t give rise to a simpler shuffle product? Unfortunately in this case, both third and fourth terms are preceded by t, which can only be eliminated at $t=0$, which are the usual MZVs. Looking closely, the last two terms replace a y with x in the word, which corresponds to some form of index addition in the multi-index. Hence these terms decrease the length of the word, and so the t-shuffle product only respects length for $t = 0$. We did not take note of this while studying the shuffle product, but this is indeed a particularly nice property of usual MZVs.

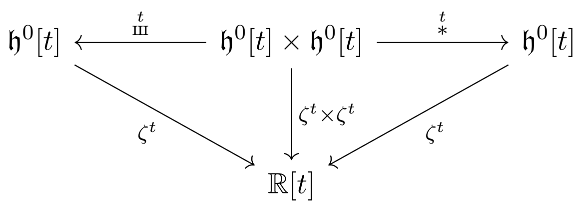
To conclude, the stuffle is particularly nice for $t = 1/2$ whereas the shuffle is particularly nice for $t = 0$, and these have no intersection. If one could somehow mix the two in order to obtain a conservation of length (either in parity or overall) in both stuffle and shuffle, then equating the two would give us an equation which splits even/odd-length zetas, a highly appealing result. Unfortunately we have not yet found a way to do this.

4.5 The t-double shuffle and regularisation

With the stuffle and shuffle products of t-zetas in hand, we are ready to generalise the double shuffle. Using our main theorems 4.3.4 and 4.4.4 and writing $\zeta^t = Z^t$, we have

$$\zeta^t(w \overset{t}{ш} w') = \zeta^t(w)\zeta^t(w') = \zeta^t(w \overset{t}{*} w')\,,$$

or in the form of a commutative diagram,



From this we conclude the t-double shuffle (t-DS) relation.

Theorem 4.5.1. For all words $w, w' \in \mathfrak{h}^0[t]$,

$$\zeta^t(w \overset{t}{ш} w' - w \overset{t}{*} w') = 0\,.$$

Remark 4.5.2. My supervisor recently pointed out that a paper [LQ] was uploaded by Li and Qin on the arXiv last year, also establishing the extended double shuffle relations for t-zetas. This paper remarks that Wakabayashi has also discovered this independently in [Wak], published while this report was being finalised. We have not read further than the introduction in each paper and our work is entirely independent of theirs, although some results and proofs will no doubt look alike.

Example 4.5.3. Taking $w = w' = z_2$, we easily get

$$w \overset{t}{*} w' = 2z_2z_2 + (1 - 2t)z_4\,.$$

From example 4.4.3,

$$w \overset{t}{ш} w' = 2z_2z_2 + 4z_3z_1 - 6tz_4\,.$$

Comparing the two, we obtain

$$(1 + 4t)\zeta^t(4) = 4\zeta^t(3, 1)\,!$$

As for usual MZVs, we ask whether this is enough to produce all $\mathbb{Q}[t]$-linear relations among t-zetas. For the same reason that we could not obtain $\zeta(2,1) = \zeta(3)$ from the DS, we cannot get $\zeta^t(2,1) = \zeta(2,1) + t\zeta(3) = (1+t)\zeta(3) = (1+t)\zeta^t(3)$ from the t-DS. [This is essentially because one of the zetas being multiplied would need to have weight 1 for the sum of weights to be 3, which does not exist].

Can we extend the t-DS through a similar process of regularisation? As for the construction of t-stuffle/shuffle, we can reduce this problem to that of MZVs.

Recall from Chapter 2 the 'filtering' function $f : (\mathfrak{h}^1, *) \longrightarrow (\mathfrak{h}^0, *)$ defined as the (unique!) homomorphism satisfying

$$f(w) = \begin{cases} w & \text{if } w \in \mathfrak{h}^0 \\ 0 & \text{if } w = y\,. \end{cases}$$

The EDS Theorem (2.5.3) stated that

$$\zeta \circ f(w_0 \,\text{ш}\, w_1 - w_0 * w_1) = 0$$

for all $w_0 \in \mathfrak{h}^0$ and $w_1 \in \mathfrak{h}^1$, where $\zeta = Z$.

We first extend the filtering function to $f : (\mathfrak{h}^1[t], *) \longrightarrow (\mathfrak{h}^0[t], *)$ by $\mathbb{Q}[t]$-linearity, remaining the unique homomorphism satisfying the two properties above. The following theorem is our generalisation of EDS to t-zetas.

Theorem 4.5.4 (t-EDS)**.** For all $w_0 \in \mathfrak{h}^0[t]$ and $w_1 \in \mathfrak{h}^1[t]$,

$$\zeta^t \circ f(w_0 \overset{t}{\text{ш}} w_1 - w_0 \overset{t}{*} w_1) = 0\,.$$

To prove it, we need the following lemma.

Lemma 4.5.5. The maps S^t and f commute.

$$\begin{array}{ccc} \mathfrak{h}^1[t] & \xrightarrow{\quad S^t \quad} & \mathfrak{h}^1[t] \\ {\scriptstyle f}\big\downarrow & \circlearrowleft & \big\downarrow{\scriptstyle f} \\ \mathfrak{h}^0[t] & \xrightarrow[\quad S^t \quad]{} & \mathfrak{h}^0[t] \end{array}$$

This makes sense since $S^t(\mathfrak{h}^0[t]) \subset \mathfrak{h}^0[t]$, which was already mentioned in previous sections. The proofs of both lemma and theorem above are given in Appendix A.4. Note that it is surprisingly straightforward to obtain the t-EDS by combining the lemma above with the usual EDS.

Example 4.5.6. Take $w_0 = z_2$ and $w_1 = z_1$. Then

$$\begin{aligned} w_0 \overset{t}{\sqcup\!\sqcup} w_1 - w_0 \overset{t}{*} w_1 &= x(y \overset{t}{\sqcup\!\sqcup} y) + yxy - txxy - (z_2z_1 + z_1z_2 + (1-2t)z_3) \\ &= x(2yy - 2txy) + z_1z_2 - tz_3 - (z_2z_1 + z_1z_2 + (1-2t)z_3) \\ &= 2z_2z_1 - 2tz_3 - z_2z_1 - (1-t)z_3 \\ &= z_2z_1 - (1+t)z_3 \,. \end{aligned}$$

In this case, the terms in $\mathfrak{h}^1[t] \setminus \mathfrak{h}^0[t]$ cancel and f acts as the identity. We conclude that

$$\zeta^t(z_2z_1 - (1+t)z_3) = 0 = \zeta^t(2,1) - (1+t)\zeta^t(3)$$

which gives the t-analogue of Euler's relation, $\zeta^t(2,1) = (1+t)\zeta^t(3)$. We learn nothing new since this comes immediately from the definition

$$\zeta^t(2,1) \coloneqq \zeta(2,1) + t\zeta(3) = \zeta(3) + t\zeta(3) = (1+t)\zeta^t(3)$$

along with Euler's relation for MZVs. But we would have found the latter relation (at least in more complicated situations) from the EDS relations, which illustrates the fact that most problems for t-zetas descend to problems for MZVs, in this case double shuffle and regularisation. Moreover, the algebraic structure is given immediately rather than going through definition, using some ad-hoc combination of the EDS and then recomposing.

Example 4.5.7. Take $w_0 = z_3$ and $w_1 = z_1$. Then

$$\begin{aligned} w_0 \overset{t}{\sqcup\!\sqcup} w_1 - w_0 \overset{t}{*} w_1 &= x(xy \overset{t}{\sqcup\!\sqcup} y) + yxxy - txxxy - (z_3z_1 + z_1z_3 + (1-2t)z_4) \\ &= x\left[x(y \overset{t}{\sqcup\!\sqcup} y) + yxy - txxy\right] + z_1z_3 - tz_4 - (z_3z_1 + z_1z_3 + (1-2t)z_4) \\ &= 2xxyy - 2txxxy + xyxy - txxxy - z_3z_1 - (1-t)z_4 \\ &= 2z_3z_1 - 2tz_4 + z_2z_2 - tz_4 - z_3z_1 - (1-t)z_4 \\ &= z_3z_1 + z_2z_2 - (1+2t)z_4 \end{aligned}$$

which yields $\zeta^t(3,1) + \zeta^t(2,2) = (1+2t)\zeta^t(4)$.

We now give a less elementary example where the function f does not act as identity.

Example 4.5.8. Take $w_0 = z_2$ and $w_1 = z_1z_1$. Then

$$\begin{aligned} w_0 \overset{t}{\sqcup\!\sqcup} w_1 &= x(yy \overset{t}{\sqcup\!\sqcup} y) + y(xy \overset{t}{\sqcup\!\sqcup} y) \\ &= x\left[y(y \overset{t}{\sqcup\!\sqcup} y) + yyy - txyy\right] + y\left[x(y \overset{t}{\sqcup\!\sqcup} y) + yxy - txxy\right] \\ &= x\left[3yyy - 2tyxy - txyy\right] + y\left[2xyy - 2txxy + yxy - txxy\right] \\ &= 3z_2z_1z_1 - 2tz_2z_2 - tz_3z_1 + 2z_1z_2z_1 - 3tz_1z_3 + z_1z_1z_2 \end{aligned}$$

and

$$\begin{aligned} w_0 \overset{t}{*} w_1 &= z_2z_1z_1 + z_1(z_2 \overset{t}{*} z_1) + (1-2t)z_3z_1 + (t^2-t)z_4 \\ &= z_2z_1z_1 + z_1z_2z_1 + z_1z_1z_2 + (1-2t)z_1z_3 + (1-2t)z_3z_1 + (t^2-t)z_4 \end{aligned}$$

which implies

$$w_0 \overset{t}{\sqcup\!\sqcup}\, w_1 - w_0 \overset{t}{*} w_1 = 2z_2z_1z_1 - 2tz_2z_2 + (t-1)z_3z_1 + z_1z_2z_1 - (t+1)z_1z_3 + (t-t^2)z_4\,,$$

which contains words in $\mathfrak{h}^1[t] \setminus \mathfrak{h}^0[t]$, which we must express as polynomials in $y = z_1$ in order to act with f. We treat each word separately:

$$\begin{aligned} z_1z_3 &= z_1 \overset{t}{*} z_3 - z_3z_1 - (1-2t)z_4 \\ z_1z_2z_1 &= z_1 \overset{t}{*} z_2z_1 - z_2(z_1 \overset{t}{*} z_1) - (1-2t)z_3z_1 - (t^2-t)z_4 \\ &= z_1 \overset{t}{*} z_2z_1 - 2z_2z_1z_1 - (1-2t)z_2z_2 + (2t-1)z_3z_1 + (t-t^2)z_4\,. \end{aligned}$$

It follows that

$$\begin{aligned} f(z_1z_3) &= -z_3z_1 + (2t-1)z_4 \\ f(z_1z_2z_1) &= -2z_2z1z_1 + (2t-1)z_2z_2 + (2t-1)z_3z_1 + (t-t^2)z_4\,. \end{aligned}$$

which implies

$$\begin{aligned} f(w_0 \overset{t}{\sqcup\!\sqcup}\, w_1 - w_0 \overset{t}{*} w_1) &= 2z_2z_1z_1 - 2tz_2z_2 + (t-1)z_3z_1 - 2z_2z_1z_1 + (2t-1)z_2z_2 + (2t-1)z_3z_1 \\ &\quad + (t-t^2)z_4 - (t+1)(-z_3z_1 + (2t-1)z_4) + (t-t^2)z_4 \\ &= (4t-1)z_3z_1 + (1+t-4t^2)z_4 - z_2z_2\,. \end{aligned}$$

Finally, the t-EDS theorem gives us the non-trivial relation

$$(4t-1)\zeta^t(3,1) + (1+t-4t^2)\zeta^t(4) = \zeta^t(2,2)\,!$$

Note that this reduces to

$$\zeta(4) = \zeta(2,2) + \zeta(3,1)$$

for usual zetas and

$$3\zeta^\star(3,1) = \zeta^\star(2,2) + 2\zeta^\star(4)$$

for star-zetas, which are not obvious either. In fact, these relations could not be attained using the DS only, so regularisation is crucial.

The following analogy helped me to better appreciate t-zetas as being entirely determined by the behaviour of usual zetas, i.e. their behaviour at $t = 0$. One way of understanding Taylor's theorem is to notice that a smooth function is fully determined by its behaviour at one point, namely the values that its (infinitely many) derivatives take at that point.

This understanding is inspired from [Yam, Chap. 5], where Yamamoto looks at *differential submodules* of $\mathfrak{h}^1[t]$ and deduces analogues of the sum theorem and cyclic sum theorem for t-zetas, which we copy without proof below.

Theorem 4.5.9 (Theorem 1.1 in Yamamoto)**.** For any integers $k > n \geq 1$, we have

$$\sum_{\substack{k_1+\ldots+k_n=k \\ k_1\geq 2,\, k_i\geq 1}} \zeta^t(k_1,\ldots,k_n) = \left(\sum_{j=0}^{n-1} \binom{k-1}{j} t^j (1-t)^{n-1-j}\right) \zeta^t(k)\,.$$

Theorem 4.5.10 (Theorem 5.4 in Yamamoto)**.** Let $n \geq 1$ and $k_1, \ldots, k_n \geq 1$ integers, and assume that $k_1, \ldots, k_n$ are not all 1. Put $k = k_1 + \ldots + k_n$. Then

$$\sum_{l=1}^{n} \sum_{j=1}^{k_l - 1} \zeta^t(k_l + 1 - j, k_{l+1}, \ldots, k_n, k_1, \ldots, k_{l-1}, j)$$
$$= (1-t) \sum_{l=1}^{n} \zeta(k_l + 1, k_{l+1}, \ldots, k_n, k_1, \ldots, k_{l-1}) + t^n k \zeta^t(k+1)\,.$$

These are entirely governed by the sum theorem and cyclic sum theorem for usual MZVs, and are in fact equivalent to them (c.f. [Yam, Remark 5.3]).

This led me to expect that conjectures about MZVs should have equivalent statements for t-zetas. I will give a few examples and results of my own below, but one should make the following crucial remark before proceeding. The reader might think: if the behaviour of t-zetas is fully determined by that of MZVs, why not reduce all problems to MZVs and study them alone?

The point is that t-zetas may *exhibit* structure that makes them preferable to work with, say at particular values like $1/2$, where the stuffle product is particularly elegant. Moreover, working with general t is stronger than any particular value, since a polynomial in t can give us potentially many relations at once, by comparing the coefficients of t^i for each i. The following example illustrates this potential.

Example 4.5.11. Take $w_0 = z_2 z_1$ and $w_1 = z_1$. Without working the example out in detail (it is almost identical to example 4.5.7 above), the t-EDS gives us

$$\zeta^t(2,1,1) = \zeta^t(2,2) + \zeta^t(3,1) + (t^2 - t)\zeta^t(4)\,.$$

Working through the same example with usual zetas (i.e. either using the usual EDS or plugging $t = 0$ above), we can obtain

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

One might think that these are entirely equivalent, and so t-zetas are rendered useless. However, this is not the case because extra relations come out of polynomial comparison. From definition, the first equation above gives us

$$\zeta(2,1,1) + t(\zeta(3,1) + \zeta(2,2)) + t^2\zeta(4) = \zeta(2,2) + t\zeta(4) + \zeta(3,1) + t\zeta(4) + (t^2 - t)\zeta(4)\,,$$

and comparing coefficients of 1 and t gives us the *two* relations

$$\zeta(2,1,1) = \zeta(3,1) + \zeta(2,2)$$
$$\zeta(3,1) + \zeta(2,2) = \zeta(4)\,,$$

which adds a relation to the usual EDS above!

Moreover, the idea of finding equivalent and analogue results for t-zetas (like the sum or cyclic theorems above) does not always work in an elegant way. Indeed, such equivalences are essentially governed through S^t, but the behaviour of S^t may not be one that respects the specific structure we are looking to preserve. For example, S^t is erratic with respect to length and results concerning length do not easily deform across t. This is testified by the fact that 1/2-MZVs have a stuffle product which respects length parity, whereas other t-zetas do not. This has to do with the corresponding submodule not being a differential submodule, because the deformation is not confined to, say, a particular length.

This highlights the possible importance of t-zetas: deformations that may preserve some types of structure but not others. Such objects are generally worth studying, often exhibiting interesting behaviour that can prove to be useful either in application or perspective. Condensing all of this to one sentence: the structure is entirely determined by that of MZVs, but it does not follow that their structures are the same.

Before moving on, we give a few interesting analogues that *do* exist wherever the operator S^t acts in a feature-preserving way. As a basic example, Zagier's conjecture is equivalent to its t-analogue, namely that there are no relations among t-zetas of different weight. This holds precisely because S^t preserves weight, and the fact that S^t is invertible allows us to claim implications both ways, i.e. equivalence. We make this precise in a more advanced scenario, namely proving the following theorem of ours.

First recall that $\bar{D} = \{f(w_0 \sqcup\!\sqcup w_1 - w_0 * w_1 \mid w_0 \in \mathfrak{h}^0, w_1 \in \mathfrak{h}^1\}$. Analogously, define $\bar{D}^t = \{f(w_0 \overset{t}{\sqcup\!\sqcup} w_1 - w_0 \overset{t}{*} w_1) \mid w_0 \in \mathfrak{h}^0[t], w_1 \in \mathfrak{h}^1[t]\}$. The t-EDS states that $\bar{D}^t \subseteq \ker(\zeta^t)$, while Conjecture 2.5.5 states

$$\bar{D} = \ker(\zeta)\,.$$

Theorem 4.5.12. The following equivalence holds:

$$\bar{D} = ker(\zeta) \quad \iff \quad \bar{D}^t = ker(\zeta^t)\,.$$

Note that from the proof of the t-EDS, we already know that the EDS and t-EDS are equivalent. This is stating something different: if the EDS generates all linear relations among MZVs, then so does the t-EDS among t-MZVs (and vice-versa). The proof is given in Appendix A.4.

Recall Conjecture 2.5.8, stating that we only need the DS + Hoffman's relation to produce all linear relations among MZVs, rather than the full EDS. We can also establish its equivalence with a t-analogue, but the process is almost identical as the one above. The DS part is identical, and the HR part follows by noticing that $S^t(y) = y$, implying

$$S^{-t}(w_0 \sqcup\!\sqcup y - w_0 * y) = S^{-t}(w_0) \overset{t}{\sqcup\!\sqcup} y - S^{-t}(w_0) \overset{t}{*} y\,.$$

Before concluding this chapter, we look at further results for t-zetas which are not as feature-preserving as the above.

4.6 Further considerations

Having established the t-analogue of the EDS, one might expect to be able to do the same for other families of relation, from duality to Ohno and derivation relations. Taking the latter as an example, this would follow if ∂_n and S^t commuted, as for f and S^t, but this does not hold. Indeed, taking $n = 2$ gives

$$S^t \circ \partial_2(y) = S^t(-x(x+y)y) = -R^t(x)R^t(x+y)y = -x(y+(t+1)x)y\,,$$

whereas

$$\partial_2 \circ S^t(y) = \partial_2(y) = -x(x+y)y\,.$$

Equality holds iff $t = 0$, which is the case of usual MZVs where the derivation relations indeed hold. Note that the case $n = 1$ does hold:

$$S^t \circ \partial_1(y) = S^t(-xy) = -xy = \partial_1(y) = \partial_1 \circ S^t(y)\,.$$

This should be expected since it corresponds to the t-analogue of Hoffman's relation, which is also a consequence of the t-EDS proven above. To make the general case hold, we define $\partial_n^t = S^{-t} \circ \partial_n \circ S^t$. Then somewhat trivially, we obtain

$$\zeta^t(\partial_n^t(w)) = \zeta(\partial_n(S^t(w))) = 0$$

for all $w \in \mathfrak{h}^0[t]$ and integer $n \geq 1$, by the derivation relations of Theorem 3.4.1. This provides us with a t-generalisation of this family, but it is only really worth having if there is an elegant expression for it. By virtue of being a derivation, the operator ∂_n is given by its simple action on x and y – but what about the operator ∂_n^t? We have

$$\begin{aligned}
\partial_n^t(y) &= S^{-t} \circ \partial_n \circ S^t(y) \\
&= S^{-t} \circ \partial_n(y) \\
&= S^{-t}(-x(x+y)^{n-1}y) \\
&= -xR^{-t}(x+y)^{n-1}y \\
&= -x(x(1-t)+y)^{n-1}y\,,
\end{aligned}$$

which is a relatively nice expression for its action on y (especially for star-zetas, at $t = 1$). Unfortunately, this operator is *not* a derivation. Omitting computations, this can be seen by looking at its action on xy, which is

$$\partial_n^t(xy) = x(x(1-t)+y)^{n-1}y^2 - (1+t)x^2(x(1-t)+y)^{n-1}y\,,$$

as opposed to

$$\partial_n^t(x)y + x\partial_n^t(y) = x(x(1-t)+y)^{n-1}y^2 - x^2(x(1-t)+y)^{n-1}y\,,$$

with equality holding only at $t = 0$. As such, it is not simple to give a description of the operator's action on a general word $w \in \mathfrak{h}^0$.

One might wish to ask the same question for duality. Similarly, define $\tau^t = S^{-t} \circ \tau \circ S^t$ and trivially obtain the t-analogue

$$\zeta^t(\tau^t(w)) = \zeta^t(w)$$

for all words $w \in \mathfrak{h}^0[t]$. For $w = z_3$ we obtain

$$\tau^t(w) = S^{-t} \circ \tau(z_3) = S^{-t}(z_2 z_1) = z_2 z_1 - t z_3\,,$$

from which the analogue of Euler's identity

$$\zeta^t(2,1) = (1+t)\zeta^t(3)$$

holds. For higher length however, the reader can easily check that the action of τ^t is not given by a simple inversion procedure as for τ. This complication gives t-duality relations which involve *more* than two zetas, thus rendering the notion of *duality* meaningless. For example, taking $w = z_2z_2$ gives

$$\begin{aligned}\tau^t(w) &= S^{-t} \circ \tau(z_2z_2 + tz_4)\\ &= S^{-t}(z_2z_2 + tz_2z_1z_1)\\ &= z_2z_2 - tz_4 + tz_2z_1z_1 - t^2(z_3z_1 + z_2z_2) + t^3z_4\,.\end{aligned}$$

Then the t-duality relation is

$$t(1-t^2)\zeta^t(4) = t\zeta^t(2,1,1) - t^2\zeta^t(3,1) - t^2\zeta^t(2,2)\,,$$

which does *not* reveal two 'dual' t-zetas.

Remark 4.6.1. Despite the failure in generalising duality to t-zetas, something interesting can still be extrapolated from t-duality, as with any relations among t-MZVs. In the case above, we have previously seen that only two MZVs are dual in weight 4, namely $\zeta(4)$ and $\zeta(2,2,1)$. Interestingly, this duality can be obtained from t-duality not only using $w = z_4$ or $w = z_2z_2z_1$ as expected, but with $w = z_2z_2$ above. Indeed, expanding the expression using the definition of t-zetas gives

$$t\zeta(4) = t\zeta(2,1,1)\,,$$

from which the relation is obtained by viewing it as a polynomial and *comparing* the coefficient of t (not evaluating it at 0).

One can perform a similar generalisation for Ohno's relation, which gives us a family of relations

$$\zeta^t(h_n^t \cdot \tau^t(w)) = \zeta^t(h_n^t \cdot w)$$

for all $w \in \mathfrak{h}^0[t]$ and integer $n \geq 0$. Once again, the expression for the above action is not elegant for general t-zetas, although they remain as powerful as the t-EDS and are expected to generate all relations among t-zetas. This is made precise by the following analogue of the Equivalence Theorem (3.4.3).

Theorem 4.6.2. The following are equivalent.

1. $\zeta^t \circ f(w_0 \overset{t}{\sqcup\!\sqcup} w_1 - w_0 \overset{t}{*} w_1) = 0$ for all $w_0 \in \mathfrak{h}^0[t]$ and $w_1 \in \mathfrak{h}^1[t]$.
2. $\zeta^t(h_n^t \cdot \tau^t(w)) = \zeta^t(h_n^t \cdot w)$ for all $w \in \mathfrak{h}^0[t]$ and integer $n \geq 0$.
3. $\zeta^t(\partial_n^t(w)) = 0$ for all $w \in \mathfrak{h}^0[t]$ and integer $n \geq 1$.

Proof. First note that we have proved the t-EDS and the EDS to be equivalent in Theorem 4.5.12, and a quasi-identical proof will show that the t-generalisations of Ohno and derivation relations are equivalent to their usual versions. As such, each of $1-3$ above are equivalent to their respective statement $1-3$ in the equivalence theorem for usual MZVs. We have seen that these are equivalent by the work of [IKZ, Theorem 3], so the proof is complete. □

In combination with Theorem 4.5.12, any of these is equivalent to the statement that the EDS generates all linear relations among (usual!) MZVs, which nicely wraps up the generalisation of all previous work to t-zetas.

We close this chapter with a conjecture of mine, stating that even-length (alternatively, even-length) t-zetas form a spanning set for t-MZVs. This idea stems from a mixture of duality (which proves this claim for odd weight and $t = 0$), and the structure behind Hoffman's relation. It originated from noticing that the half-stuffle preserves length parity. The half-shuffle does not, although it only produces two possible lengths: the sum of both arguments and one less. As such, we can imagine that it may be possible to express all even (or odd) half-zetas in terms of the remaining, which are all of opposite parity. The half-version of Hoffman's relation gives a particularly nice formula, and we think that it might allow us to express all odd half-zetas in terms of even ones. For usual zetas, the shuffle is particularly nice for $t = 0$, and the stuffle is also elegant in terms of length in Hoffman's relation, although not in general. As such, this also seems to work for usual zetas. We give an example before stating the conjecture.

Example 4.6.3. We reduce all odd-length half-zetas to even ones for weight $k = 4$. Example 4.5.7 gives us Hoffman's relation

$$2\zeta^{\frac{1}{2}}(4) = \zeta^{\frac{1}{2}}(3,1) + \zeta^{\frac{1}{2}}(2,2)$$

for $w_0 = z_3$, as required to eliminate $\zeta^{\frac{1}{2}}(4)$. Now $w_0 = z_2 z_1 = xyy$ gives

$$\begin{aligned} w_0 \overset{t}{\text{Ш}} y - w_0 \overset{t}{*} y &= x(yy \overset{t}{\text{Ш}} y) + yxyy - txxyy - z_1 z_2 z_1 - 2z_2 z_1 z_1 \\ &= x\left[y(y \overset{t}{\text{Ш}} y) + yyy - txyy\right] - tz_3 z_1 - 2z_2 z_1 z_1 \\ &= x\left[3yyy - 2tyxy - txyy\right] - tz_3 z_1 - 2z_2 z_1 z_1 \\ &= z_2 z_1 z_1 - 2tz_2 z_2 - 2tz_3 z_1\,, \end{aligned}$$

which yields

$$\zeta^{\frac{1}{2}}(2,1,1) = \zeta^{\frac{1}{2}}(3,1) + \zeta^{\frac{1}{2}}(2,2)$$

as required to eliminate $\zeta^{\frac{1}{2}}(2,1,1)$, and so we have eliminated all odd-length half-zetas. The reader is encouraged to do the same for weight $k = 5$, where we cannot eliminate them one by one but instead must use linear combinations of the relations we obtain.

Conjecture 4.6.4. For any $t \in \mathbb{R}$, the set of even-length t-zetas is a spanning set for all t-zetas. Moreover, Hoffman's relation is enough to express all odd-length t-zetas in terms of even ones, at least for $t = 0$ and $t = 1/2$.

To support the first half of this conjecture, we constructed the set of even-length zetas inductively by constructing an appropriate program in PARI/GP, and verifying that some subset forms a numerical basis for $t = 0$ and $t = 1/2$, up to weight $k = 15$, with a precision of 3,000 digits.

Chapter 5

Motivic MZVs: beyond numbers

This chapter is written in a slightly more wordy way than the previous ones, bearing in mind newcomers in the field. The more experienced reader will be capable of engaging directly with the papers I reference.

5.1 Introduction

The previous chapters focused on exploring the immense wealth of relations among MZVs and their interpolation. A standard mathematical way of condensing the information that relations provide, is to express all elements in terms of a selected few. This is precisely the idea of a *spanning set*, and the dimension of the vector space $\mathcal{Z}_k$ will be bounded by the size of that set. Proving linear independence turns it into a *basis*, in which case the bound becomes equality. In our case, we would like to express all MZVs in terms of a selected few through the EDS (or an equivalent family), and the conjecture that the EDS provides all relations would imply obtaining a basis. Unfortunately, we have seen that even bounding the dimension of $\mathcal{Z}_k$ by d_k using such a family is out of reach for now, because many of the relations may intersect in an unpredictable way, thus giving linearly dependent ('duplicate') relations.

However, a new approach based on the theory of motives has proven very powerful in both bounding the dimension, and more recently given rise to an explicit spanning set. Showing that the elements are linearly independent is out of reach for now, but the result cannot be underestimated in both strength and difficulty. This final chapter aims to give a quick glimpse of the ideas that have contributed to this approach. We begin by recalling the main results which have stemmed from this theory, as stated in Section 1.4.

Recall Hoffman's family

$$B = \{\zeta(s_1, \dots, s_r) \mid s_i \in \{2, 3\}$$

and

$$B_k = \{\zeta(s_1, \dots, s_r) \mid s_i \in \{2, 3\},\, wt(s_1, \dots, s_r) = k\} = B \cap \mathcal{Z}_k$$

for $k \geq 2$, with $B_0 \coloneqq \{1\}$ and $B_1 \coloneqq \{0\}$.

Theorem 5.1.1 (Terasoma and Deligne-Goncharov)**.** For all $k \geq 0$,

$$\dim_{\mathbb{Q}}(\mathcal{Z}_k) \leq d_k \,.$$

Hoffman's Conjecture. B_k is a $\mathbb{Q}$-basis for $\mathcal{Z}_k$.

The major recent breakthrough was achieved by Brown, proving the 'spanning' half of this conjecture.

Brown's Theorem. Any MZV can be written as a $\mathbb{Q}$-linear combination of $\zeta(s_1, \ldots, s_r)$ with $s_i \in \{2, 3\}$ for all i. In other words,

$$\operatorname{span}_{\mathbb{Q}}\{B_k\} = \mathcal{Z} \,.$$

By Proposition 1.4.9, Brown's Theorem implies $\dim_{\mathbb{Q}}(\mathcal{Z}_k) \leq |B_k| = d_k$, so Theorem 5.1.1 is its corollary. Moreover, Hoffman's family will form a basis for $\mathcal{Z}_k$ if Zagier's conjecture holds.

5.2 Periods

5.2.1 Naïve periods

The second section introduces periods, a class of complex numbers $\mathcal{P}$ which is strictly contained between algebraic and transcendental numbers. We will see that MZVs belong to $\mathcal{P}$, and that periods exhibit further algebraic structure which underlie the motivic approach. We reproduce in our own words the introductory pages of Kontsevich and Zagier's survey article [KZ], where periods were first defined. For the curious reader we highly recommend the article as an elegant, accessible and well-motivated piece of work, building bridges between this class of numbers and many areas of mathematics. We first recall the definition of algebraic numbers.

Definition 5.2.1. An algebraic number is any complex root of a non-zero polynomial in one variable with rational coefficients. More precisely, $a \in \mathbb{C}$ is an algebraic number iff there exists $0 \neq f \in \mathbb{Q}[x]$ such that $f(a) = 0$.

Note that we can consider only polynomials with integer coefficients by multiplying f with the product of all coefficient denominators, which does not affect its roots. We call a number $a \in \mathbb{C}$ transcendental if a is not algebraic.

Two important properties of algebraic numbers is that are countable and form an algebraically closed field denoted $\overline{\mathbb{Q}}$, the algebraic closure of rational numbers.

Examples 5.2.2.

1. Any rational number $q \in \mathbb{Q}$ is algebraic, as the root of $f(x) = x - q$.
2. For any $n \geq 1$, the nth root of a number $q \in \mathbb{Q}$ is algebraic, as the root of $f(x) = x^n - q$.
3. Both e and π are *not* algebraic. Indeed, the special case $n = 1$ of the Lindemann-Weierstrass theorem states that if a is algebraic then e^a is transcendent, so taking $a = 1$ gives the result for e. Assuming that π is algebraic gives πi also algebraic, so that $e^{\pi i} = 1$ is transcendent, a contradiction.

These examples give us strict inclusions $\mathbb{Q} \subset \overline{\mathbb{Q}} \subset \mathbb{C}$, and we copy the diagram from KZ classifying complex numbers as follows:

$$\begin{array}{ccccccc} \mathbb{N} & \subset & \mathbb{Z} & \subset & \mathbb{Q} & \subset & \overline{\mathbb{Q}} \\ & & & & \cap & & \cap \\ & & & & \mathbb{R} & \subset & \mathbb{C} \end{array} .$$

We could also have written $\mathbb{C} = \overline{\mathbb{R}}$, since the algebraic closure of $\mathbb{R}$ is $\mathbb{C}$ by the fundamental theorem of algebra. Note that the sets in the first row are all countable whereas those in the second are not. In this sense, 'almost all' complex numbers are transcendent, and the gap between algebraic and complex is immense. We will see that periods are somewhat more ambiguous, and give rise to deep mathematical structure which we explore in the next section.

Definition 5.2.3 (Kontsevich-Zagier)**.** A period is a complex number whose real and imaginary parts are values of absolutely convergent integrals of rational functions with rational coefficients, over domains in $\mathbb{R}^n$ given by polynomial inequalities with rational coefficients.

More precisely, a number $p \in \mathbb{C}$ is a period iff there exist polynomials f and $g \neq 0$ in $\mathbb{Q}[x_1, \dots, x_n]$ such that

$$p = \int_\Delta \frac{f(x_1, \dots, x_n)}{g(x_1, \dots, x_n)}\, dx_1 \dots dx_n \,.$$

where $\Delta \subset \mathbb{R}^n$ is a domain given by finite unions and intersections of regions $\{(x_1, \dots, x_n) \in \mathbb{R}^n \mid h(x_1, \dots, x_n) \geq 0\}$ with $h \in \mathbb{Q}[x_1, \dots, x_n]$.

Examples 5.2.4.

1. Rational numbers are trivially periods (take the rational number as integrand and $0 \leq x \leq 1$ as domain). It follows that i is a period since its real and imaginary parts are 0 and 1.

2. The number $\sqrt{2}$ is a period since

$$\int\limits_{0 \leq x^2 \leq 2} dx = \int\limits_0^{\sqrt{2}} dx = \sqrt{2} \,.$$

3. The numbers above are also algebraic. What about non-algebraic periods? Consider the integral

$$\int\limits_{x^2+y^2=1} dxdy \,.$$

Make the change of variables $x = r\cos\theta$ and $y = r\sin\theta$, with Jacobian

$$\det \begin{pmatrix} \cos\theta & \sin\theta \\ -r\sin\theta & r\cos\theta \end{pmatrix} = r \,.$$

Then

$$\int\limits_{x^2+y^2=1} dxdy = \int_0^1 \int_0^{2\pi} r\, d\theta dr = 2\pi \left[\frac{r^2}{2}\right]_0^1 = \pi \,,$$

so π is a period.

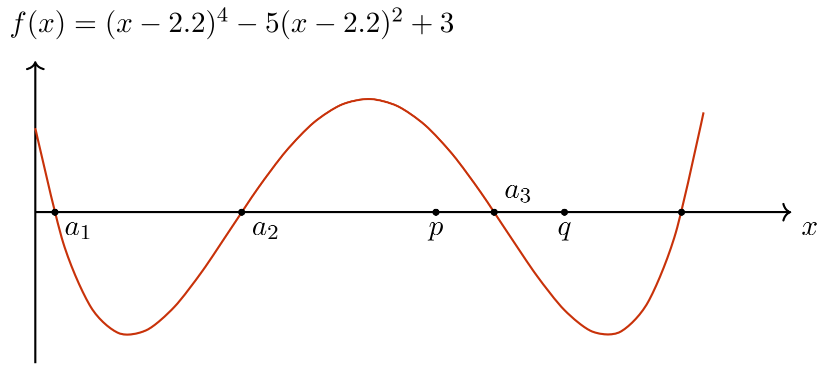
4. The logarithm of a rational number q is a period since
$$\int_{1\leq x\leq q} \frac{dx}{x} = \log(q)\,.$$
5. Elliptic integrals, special values of modular forms, various L-functions attached to them and particular powers of rational values of the gamma function are also periods, details of which can be found in [KZ].
6. It is conjectured that e, $1/\pi$ and Euler's constant γ are *not* periods, but this is unproved.

The following proposition is assumed in KZ, and gives meaning to the idea that periods bridge some of the gap between algebraic and complex numbers.

Proposition 5.2.5. All algebraic numbers are periods.

Exceptionally, we include an original but rather long proof in the main body. Nowhere have we found the sketch of a proof, which was exciting to discover.

Proof. First take any *real* algebraic number a. We prove the claim for $a > 0$, from which the negative case will follow. By definition, there exists $0 \neq f \in \mathbb{Q}[x]$ such that $f(a) = 0$, and we take this polynomial to have *minimal* degree. Then f' has degree strictly smaller than f, so we cannot have $f'(a) = 0$. Let $\{a_1, \ldots, a_r\}$ the *real* roots of f such that $0 < a_i \leq a$ for all i, and order them in an increasing order, so that $a_1 \leq \ldots \leq a_r = a$. Also define $a_0 = 0$, and notice that $a_{r-1} < a_r$ since $a_r > 0$ and $a_{r-1} = a_r$ implies that f has a double root at a, which in turns implies $f'(a) = 0$, a contradiction. Now let
$$D_i = \{x \mid a_{i-1} < x < a_i\}$$
for each $1 \leq i \leq r$. Note that f has constant sign in each domain D_i, since f continuous implies that it can only change sign by taking value 0, but this never happens in D_i since $a_j \notin D_i$ for all j. Note also that D_r is non-empty since $a_r > a_{r-1}$. Since the rationals are dense in $\mathbb{R}$, we can find $p \in \mathbb{Q}$ such that $a_{r-1} < p < a_r$. As such, let
$$s = \text{sign}(f(D_r)) = \text{sign}(f(p))\,.$$
Now $f'(a) \neq 0$ implies that f changes sign at a. More precisely, there exists $\epsilon > 0$ such that $\text{sign}(f(a+\delta)) \neq s$ for all $\delta < \epsilon$. The rationals are dense in $\mathbb{R}$, so we can find $q \in \mathbb{Q}$ such that $a < q < a + \epsilon$. We visualise this with $a = a_3$ the root of a constructed quartic function f.



Finally, consider the domain

$$\Delta = \Big(\{x \mid sf(x) \geq 0\} \cap \{0 \leq x \leq q\}\Big) \cup \Big(\{x \mid sf(x) \leq 0\} \cap \{0 \leq x \leq p\}\Big)\,,$$

which satisfies the conditions of being defined by finite unions and intersections of rational regions, as in the definition of a period. Now note that $a < x < q$ implies $\operatorname{sign}(sf(x)) = s \cdot \operatorname{sign}(f(x)) \neq s \cdot s = 1$, so $sf(x) < 0$. Similarly, $p < x < a$ implies $sf(x) > 0$ and the domain becomes

$$\begin{aligned}\Delta &= \Big\{x \mid sf(x) \geq 0\} \cap \{0 \leq x \leq a\}\Big) \cup \Big(\{x \mid sf(x) \leq 0\} \cap \{0 \leq x \leq a\}\Big) \\ &= \{0 \leq x \leq a\}\,.\end{aligned}$$

Finally, we obtain

$$\int_\Delta dx = \int_0^a dx = a$$

with the domain as required and the integrand being the rational function 1, so a is indeed a period.

If $a < 0$, consider $-a > 0$ and find appropriate domain Δ as above such that

$$\int_\Delta dx = -a\,.$$

Then we immediately obtain that a is also a period, since -1 is also rational and

$$\int_\Delta -dx = a\,.$$

Finally, take a any *complex* algebraic number. Then $a = b + ci$ for some $b, c \in \mathbb{R}$, and there exists $0 \neq f \in \mathbb{Q}[x]$ such that $f(a) = 0$. The coefficients of f are rational, therefore real, so we have $\bar{f} = f$. This implies $f(\bar{a}) = \overline{f(a)} = \bar{0} = 0$, so $\bar{a}$ is also algebraic. Since the set of algebraic numbers forms a field with $2, i \in \overline{\mathbb{Q}}$, we obtain

$$b = \frac{a + \bar{a}}{2} \in \overline{\mathbb{Q}} \qquad \text{and} \qquad c = \frac{a - \bar{a}}{2i} \in \overline{\mathbb{Q}}\,.$$

Both b and c are now *real* algebraic numbers, and therefore periods by the previous argument. By definition, a is also a period since its real and imaginary parts are periods. □

Note that $\mathcal{P}$ is easily seen to form a ring. It is also countable, and each element can be described by a finite amount of information (the integrand and domain of integration), which is true of algebraic but not of transcendental numbers in general. However, periods strictly contain algebraic numbers, appear ubiquitously across mathematics (in particular with π and logarithms), and a period may have many distinct representations. For instance,

$$\int\limits_{\{x \geq 0\} \cup \{x \leq 0\}} \frac{dx}{1 + x^2} = \int\limits_{-\infty}^{\infty} \frac{dx}{1 + x^2} = \lim_{x \to \infty} [\arctan(x) - \arctan(-x)] = \pi\,,$$

which represents the period π in two distinct ways:

$$\int\limits_{x^2+y^2=1} dxdy = \pi = \int\limits_{x\in\mathbb{R}} \frac{dx}{1+x^2} \ .$$

As a result, it may not be clear whether two periods given by explicit integrals are equal or different, which points to their complexity. This will be crucial to our understanding of MZVs as objects with more structure than mere numbers.

But what does this have to do with MZVs at all? Well, a direct application of Kontsevich's integral representation is that all MZVs are periods. Indeed, for any multi-index $\mathbf{a}$ with weight n and binary form $\bar{\mathbf{a}} = \epsilon_1 \dots \epsilon_n$, we have

$$\zeta(\mathbf{a}) = \int_{\Delta^n} \omega_{\epsilon_1} \dots \omega_{\epsilon_n} \ .$$

The domain of integration is $\Delta^n = \{1 > t_1 \dots > t_n > 0\}$ and the integrand is a finite product of the rational functions $1/t$ and $1/(1-t)$, so all MZVs are periods. For example,

$$\zeta(2) = \int\limits_{1>t_1>t_2>0} \frac{dt_1 dt_2}{t_1(1-t_2)} \ .$$

We will name the periods as defined above *naïve* periods, for a reason soon to be made clear.

Remark 5.2.6. In the definition of periods, one might ask why we consider rational functions and rational coefficients in the polynomials rather than algebraic functions and coefficients. The answer is that we can indeed replace 'rational' with 'algebraic' everywhere in the definition, but it turns out that we obtain the same class of numbers. This comes from the fact that algebraic numbers are periods, so we can write an algebraic function $f(x_1, \dots, x_n)$ as the integral of a rational function $g(y_1, \dots y_m)$, with domain given by polynomial inequalities with coefficients now being *rational combinations of* $x_1, \dots x_n$.

Therefore, at the price of introducing more variables (which is irrelevant in our definition of periods), we can write the algebraic function over an algebraic domain as the integral of a rational function over a rational domain, and therefore obtain the same class of numbers.

5.2.2 Cohomological periods

The information that periods contain, in the form of an integral over an algebraic domain, turns out to be of rich and useful geometric nature. As such, a second way of understanding periods is through the tools of algebraic geometry and topology. This section aims to give the reader a preview of MZVs (periods) as objects appearing in the language of cohomology on algebraic varieties. This more sophisticated approach suggests that MZVs (periods) are endowed with further algebraic meaning, or structure. More precisely, periods appear as a comparison between two widely used cohomology theories, namely singular (also called Betti) and de Rham.

Unfortunately we will not be able to expose the topic in depth, instead giving simply a glimpse of how MZVs can be viewed in this light. Luckily, the book [BGF] in preparation is written on precisely this topic. A good portion of this subsection is inspired and moreover made clearer with the help of Dr. Fresán, who I thank warmly for his support. His detailed answers to a few questions were of invaluable help, along with sending me a copy of the book. We try nonetheless to give my own limited perspective of the topic and expose the introductory material in a fresh, accessible way.

To begin, we refer to the Appendix for ground-level knowledge in algebraic geometry and topology. We have re-written any content that requires modern/advanced algebraic geometry in an elementary way, so as to avoid further requirements from the reader. With this in hand, we give a definition of cohomological periods, which varies slightly according to source. We vaguely follow [KZ] but were obliged to make drastic simplifications, at the cost of losing the full definition and generality. We consider differential forms instead of their algebraic version, strictly non-relative homology, and take $\mathbb{Q}$ instead of a more general subfield $k \subseteq \mathbb{C}$.

Definition 5.2.7 (KZ)**.** Let X be a smooth algebraic variety, ω a closed differential n-form on X, all defined over $\mathbb{Q}$. Finally, let σ a singular n-chain on $X(\mathbb{C})$. Then the integral

$$p = \int_\sigma \omega$$

is called a cohomological period.

Example 5.2.8. The results stated here are from Examples B.2.1 and B.3.2 of the Appendix. Let X be the affine variety given by the polynomial $f(x, y) = xy - 1 \in \mathbb{Q}[x, y]$. We have shown that the set of complex points is $M := X(\mathbb{C}) = \mathbb{C} \setminus \{0\}$. The singular 1-chain $\sigma_1 : \Delta^1 \longrightarrow M$ is given by

$$\sigma_1(t, 1 - t) = e^{2\pi i t}\,,$$

and ω is the differential 1-form

$$\omega = \frac{dx}{x}$$

on X. It is closed since $d : E^1(X) \longrightarrow E^2(X)$, but there are no 2-forms. Then a first course in complex analysis will yield

$$p = \int_{\sigma_1} \omega = 2\pi i$$

from Cauchy's integral formula, which implies that $2\pi i$ is a cohomological period.

There is a further, even more sophisticated definition. It comes about through Gröthendieck's comparison isomorphism, first formulated in [Gro, Theorem 1]. We present it following [BGF, Theorem 2.34].

Theorem 5.2.9 (Gröthendieck)**.** Let X be a smooth algebraic variety over $\mathbb{Q}$. Then there is a canonical isomorphism

$$\text{comp} : H^i_{dR}(X) \otimes_{\mathbb{Q}} \mathbb{C} \longrightarrow H^i_B(X) \otimes_{\mathbb{Q}} \mathbb{C}$$

If X is an affine variety, the comparison isomorphism is induced by the pairing

$$H^i_{dR}(X) \otimes H_i(X(\mathbb{C}), \mathbb{Q}) \longrightarrow \mathbb{C}$$
$$[\omega] \otimes [\sigma] \longmapsto \int_\sigma \omega\,.$$

One must check that the pairing is independent of our choice of class representatives σ and ω. This follows from Stokes' theorem, although we do not give further details here.

Remark 5.2.10. What do we really mean by the isomorphism being 'induced' by this pairing? Working with rational coefficients, the singular homology and cohomology *over* $\mathbb{Q}$ are dual to each other by virtue of the universal coefficient theorem. More precisely, we have

$$H^i_B(X) \cong \mathrm{Hom}(H_i(X(\mathbb{C}), \mathbb{Q}), \mathbb{Q})\,,$$

with a bijection between generators of $H_i(X(\mathbb{C}), \mathbb{Q})$ and $H^i_B(X)$ sending σ to σ^*. Then the comparison isomorphism is given by the pairing

$$[\omega] \otimes [\sigma] \longmapsto \int_\sigma \omega\,,$$

in the sense that

$$\mathrm{comp}([\omega]) = \sum_{\sigma^*} \left(\int_\sigma \omega\right) [\sigma^*]$$

where the sum runs over all generators σ^* of $H^i_B(X)$.

Another way to write the pairing to define the vectors $\mathbf{w}$ and $\mathbf{z}$ whose entries are the generators $[\omega_n]$ and $[\sigma^*_m]$ of $H^i_{dR}(X)$ and $H^i_B(X)$ respectively, which have the same size k since comp is an isomorphism. If X is affine, we moreover define the matrix C as

$$C_{nm} = \int_{\sigma_m} \omega_n$$

and the theorem states that

$$\mathrm{comp}(\mathbf{w}) = C\mathbf{z}\,,$$

or coming back to the original form,

$$\mathrm{comp}([\omega_n]) = \sum_{m=0}^{k} C_{nm}[\sigma^*_m]\,.$$

Note that we have left complexification (tensoring with $\mathbb{C}$) implicit for simplicity. Although we may not have such an explicit matrix in the non-affine case, the isomorphism can still be represented (as all linear maps can) by a matrix C. Then the more sophisticated definition of periods is as follows.

Definition 5.2.11. A cohomological period is any entry of the matrix C representing comp for some smooth algebraic variety X over $\mathbb{Q}$.

We are cheating here since this should be defined for any *pair* (X, Z) and the relative version of Gröthendieck's comparison isomorphism. We leave it as is for simplicity. It is easy to see that the two definitions of cohomological periods are equivalent for affine varieties, since the entries of the matrix are precisely elements of the form

$$\int_\sigma \omega \,,$$

as for the first definition. This is not obvious in general. The crucial point here is that we must tensor the Betti and de Rham cohomologies with $\mathbb{C}$ to obtain a *canonical* isomorphism. The vector spaces $H^i_{dR}(X)$ and $H^i_B(X)$ are still isomorphic since they are of the same dimension over $\mathbb{Q}$, but the canonical feature is lost. In the words of [BGF, p. 78], "the fact that the comparison isomorphism does not respect the rational structures gives rise to the *periods*". In this new light, periods measure how far the rational structures of algebraic varieties are from being preserved, which endows them with further algebraic subtlety than simple numbers.

Example 5.2.12. Take X, M as in Example 5.2.8 above. From Examples B.2.1 and B.3.2 of the Appendix, we know that de Rham cohomology is given by

$$H^i_{dR}(X) = \begin{cases} \mathbb{Q} & \text{if } i = 0 \\ \mathbb{Q}(\omega) & \text{if } i = 1 \\ 0 & \text{else,} \end{cases}$$

where $\omega = \frac{dt}{t}$. We also obtained the singular homology

$$H_i(M, \mathbb{Q}) = \begin{cases} \mathbb{Q}(\sigma_0) & \text{if } i = 0 \\ \mathbb{Q}(\sigma_1) & \text{if } i = 1 \\ 0 & \text{else,} \end{cases}$$

where σ_0, σ_1 are the singular chains on M given by

$$\sigma_0(1) = 1$$
$$\sigma_1(t, 1-t) = e^{2\pi i t} \,.$$

Then the isomorphism comp for $i = 1$ is induced by the pairing

$$[\omega] \otimes [\sigma_1] \mapsto \int_{\sigma_1} \omega = 2\pi i \,,$$

so that the comparison isomorphism is given by

$$\text{comp}([\omega]) = 2\pi i [\sigma^1] \,.$$

It follows that $2\pi i$ is a cohomological period, manifesting as the entry of the one-dimensional matrix $C = (2\pi i)$.

Proposition 5.2.13. The set of cohomological periods (as defined by *either* of the above) is equal to that of naïve periods, so all three definitions are equivalent.

This proposition is highly non-trivial, but KZ give a rough explanation of why it holds, as follows: "the reason is that we can deform γ to a semi-algebraic chain and then break it up into small pieces which can be projected bijectively onto open domains in $\mathbb{R}^n$ with algebraic boundary". Although much too technical for us, a formal proof can be found in Benjamin Friedrich's thesis [Fri, Period Theorem 7.1.1].

However, given a naïve period p with explicit integral representation, it is in general very hard to find a pair (X, Z) such that p is its cohomological period. The proposition states that such a pair must exist, but the proof is not constructive.

Example 5.2.14. Having already seen that MZVs are naïve periods, we give an indication as to how $\zeta(2)$ can be exhibited as a cohomological period. This will give an idea of the difficulties encountered when displaying the required algebraic variety explicitly. We initially worked through this ourselves with inspiration from [BGF, Example 2.4.1] and previous knowledge of blow-up learnt in an undergraduate course, but decide to give only an indication and refer to BGF for a rigorous treatment. It would otherwise require more knowledge of algebraic geometry than we can introduce in this report.

Recall that Kontsevich's formula gives us the representation

$$\zeta(2) = \int_{1 \geq t_1 \geq t_2 \geq 0} \frac{dt_1 dt_2}{t_1(1-t_2)} .$$

It is thus natural to choose the domain of integration to be the singular 2-chain

$$\sigma = \{(t_1, t_2) \in \mathbb{A}^2 \mid 1 \geq t_1 \geq t_2 \geq 0\} \subset \mathbb{A}^2 ,$$

where $\mathbb{A}^2$ is the affine plane over $\mathbb{R}$. Then we can write the integrand as the differential form

$$\omega = \frac{dt_1}{t_1} \wedge \frac{dt_2}{1-t_2} \in \Omega^2(\mathbb{A}^2)$$

on $\mathbb{A}^2$. The immediate issue we face is that ω is singular along the lines

$$l_0 = \{t_1 = 0\} \qquad \text{and} \qquad l_1 = \{t_2 = 1\} ,$$

so that ω is only a non-singular differential 2-form on $Y = \mathbb{A}^2 \setminus (l_0 \cup l_1)$. We want to consider the integral of ω over σ, but σ is not contained in Y since $(0, 0) \in \sigma$ but $(0, 0) \notin Y$, and similarly for $(1, 1)$. One can overcome this problem through a technique called *blow-up*, which aims to remove this singularity by introducing projective lines $\mathbb{P}^1$ and replacing the problematic points with so-called *exceptional divisors*. More precisely, the blow-up along $(0, 0)$ and $(1, 1)$ is the projective subvariety $X \subset \mathbb{A}^2 \times \mathbb{P}^1_1 \times \mathbb{P}^1_2$ defined by

$$t_1\alpha_1 = t_2\beta_1$$
$$(t_1 - 1)\alpha_2 = (t_2 - 1)\beta_2$$

where $[\alpha_i : \beta_i]$ are homogeneous coordinates of $\mathbb{P}^1_i$. We can then project back to $\mathbb{A}^2$ through a map $\pi : X \longrightarrow \mathbb{A}^2$ by eliminating the projective components. We do not go into more detail, but this eventually leads to a resolution of singularity. One further problem arises in BGF, namely that σ is *not* a closed chain, but eventually we obtain $\zeta(2)$ as a cohomological period with a *blown-up* differential form and singular chain.

For general MZVs, it is very difficult to exhibit a differential form and singular chain which turns the MZV into a cohomological period. Goncharov and Manin accomplished this task in [GM], stating that $\zeta(\mathbf{a})$ of weight n is a period of some 'moduli space' $\mathcal{M}_{0,n+3}$.

5.3 Motivic iterated integrals and coproduct

It turns out that viewing MZVs as (cohomological) periods gives rise to deeper structure than simple numbers can provide. This culminates in 'lifting' or 'upgrading' MZVs to *motivic* MZVs, as initiated by Goncharov. Although we are unable to give a description of what motives even *are*, this section gives an intuition for them. The surprising fact is that we can still appreciate and work in the given framework to some extent, despite knowing little about what the symbols mean. I am very skeptical about performing such blind manipulations, but this works well as a concluding chapter to spark both curiosity and understanding of the theory's potency. Moreover, we explain the origin of the relations and ideas we encounter as best as possible, and give our own proofs for results left to the reader in papers.

Remark 5.3.1. Note that Kontsevich's insight in formulating MZVs as integrals (and thus as periods) is crucial to this entire theory, for algebraic geometry is very much concerned with integrals rather than sums. Deligne himself writes:

> Alors que la notion de somme infinie est étrangère à la géométrie algébrique, l'étude d'intégrales de quantités algébriques en est une des sources. C'est grâce à la [formulation de Kontsevich] que la géométrie algébrique, plus précisément la théorie des motifs de Tate mixte, est utile à l'étude des nombres multizêtas. [Del, p. 3]

I provide my own translation as follows:

> Whereas the notion of infinite sum is foreign to algebraic geometry, the study of integrals of algebraic quantities is one of its roots. It is thanks to [Kontsevich's formulation] that algebraic geometry, more precisely the theory of mixed Tate motives, is useful to the study of multiple zeta values.

We begin by introducing a powerful coproduct that Goncharov defined on motivic iterated integrals in [Gon], a special case of which are motivic MZVs.

Definition 5.3.2 (Goncharov)**.** Define the iterated integral

$$I_\gamma(a_0; a_1, \ldots, a_n; a_{n+1}) = \int\limits_{\Delta_{n,\gamma}} \frac{dt_1}{t_1 - a_1} \wedge \ldots \wedge \frac{dt_n}{t_n - a_n}$$

where γ is a path from a_0 to a_{n+1} in $\mathbb{C} \setminus \{a_1, \ldots, a_n\}$ and integration is over a simplex $\Delta_{n,\gamma}$ consisting of all ordered n-tuples of points $(t_1, \ldots, t_n)$ on γ. Note that there is no restriction on the values of a_i, so the integral may be divergent. Goncharov states in [Gon, p.1] that a regularisation/extension procedure allows us to study these objects regardless. Moreover, it is proved in [Gon, p. 2] that this does not depend on our choice of path γ, so we can remove it.

We make precise the case where this integral corresponds to an MZV. This happens when $a_0 = 0$, $a_{n+1} = 1$, γ is the straight line from 0 to 1, all a_i are in $\{0, 1\}$ and the simplex is $\Delta_{n,\gamma} = \Delta^n = \{1 > t_1 > \ldots > t_n > 0\}$. Then Kontsevich's formula gives us that for a multi-index $\mathbf{a}$ with binary form $\bar{\mathbf{a}} = a_1 \ldots a_n$, we have

$$\zeta(\mathbf{a}) = \int_{\Delta^n} \frac{(-1)^{a_1} dt_1}{t_1 - a_1} \cdots \frac{(-1)^{a_n} dt_n}{t_n - a_n} = (-1)^{l(\mathbf{a})} I_\gamma(0; a_1, \ldots, a_n; 1)\,.$$

Note that taking the wedge product or omitting it is the same here, since we have oriented the simplex positively. As a consequence, the iterated integral is our usual MZV up to a sign difference. For the rest of this section we work with general iterated integrals, but their relevance to us is the case of MZVs in binary form.

The crucial remark in Goncharov's paper is that these numbers are "periods of $\mathbb{Q}$-rational framed Hodge-Tate structures", and that the coproduct of the associated Hopf algebra (given below) is "something really new: it is invisible on the level of numbers". If the parameters a_i above are algebraic numbers (which they are for MZVs since $a_i \in \{0, 1\}$), we can do even better and upgrade the iterated integral above to a "framed mixed Tate motive over $\overline{\mathbb{Q}}$" called *motivic iterated integral*, denoted by

$$I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1})\,.$$

Let $\mathcal{H}$ the space of motivic iterated integrals. If all $a_i \in \{0, 1\}$, we call this object a *motivic MZV* and denote their subspace $\mathcal{M} \subset \mathcal{H}$. The reader can simply view these motivic integrals as formal objects which are given some algebraic structure. They should however keep in mind that they resemble integrals, to better understand the origin of later relations. All we need to know is that it lies in a commutative, graded Hopf Algebra $\mathcal{H}$ with shuffle product $\sqcup\!\sqcup$ behaving as for MZVs, and some coproduct Δ.

Proposition 5.3.3. Motivic iterated integrals satisfy the shuffle product formula

$$I^{\mathfrak{m}}(a; a_1, \ldots, a_n; b) I^{\mathfrak{m}}(a; a_{n+1}, \ldots, a_{n+m}; b) = \sum_{\sigma \in \mathrm{Sh}(n,m)} I^{\mathfrak{m}}(a; a_{\sigma(1)}, \ldots, a_{\sigma(n+m)}; b)\,.$$

We now define the period map per : $\mathcal{H} \longrightarrow \mathbb{C}$ as

$$\mathrm{per}(I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1})) = I(a_0; a_1, \ldots, a_n; a_{n+1})\,,$$

which 'descends' motivic integrals into integrals, namely numbers in $\mathcal{P}$. This map is surjective, which explains why we say that MZVs are 'lifted' or 'upgraded' to motivic MZVs.

An important feature of Goncharov's paper is that the coproduct on such objects can be computed by an explicit, visual formula.

Theorem 5.3.4. [Gon, Theorem 1.2] The coproduct $\Delta : \mathcal{H} \longrightarrow \mathcal{H} \otimes \mathcal{H}$ is given by

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

where $0 \leq k \leq n$ and $a_i \in \overline{\mathbb{Q}}$. Moreover, the terms in this formula are in bijection with the subsequences

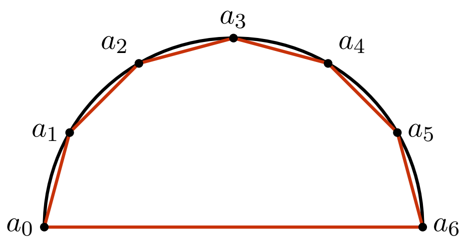
$$\{a_{i_1}, \ldots, a_{i_k}\} \subset \{a_1, \ldots, a_n\} .$$

If we locate the ordered sequence $\{a_0, \ldots, a_{n+1}\}$ on a semicircle, then the terms correspond to the polygons with vertices at the points a_i, containing a_0 and a_{n+1}, inscribed into the semicircle.

We illustrate this for two chosen terms of the case $n = 5$. The term

$$I^{\mathfrak{m}}(a_0; a_1, \ldots, a_5; a_6) \otimes 1$$

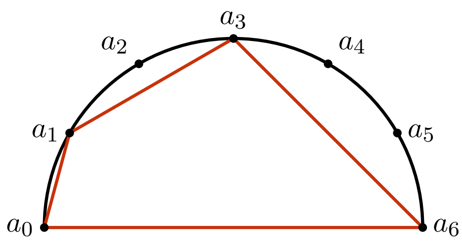
corresponds to the polygon with vertices $\{a_0, \ldots, a_6\}$:



The more elaborate term

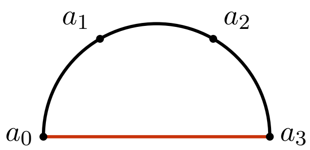
$$I^{\mathfrak{m}}(a_0; a_1, a_3; a_6) \otimes I^{\mathfrak{m}}(a_0; a_1) I^{\mathfrak{m}}(a_1; a_2; a_3) I^{\mathfrak{m}}(a_3; a_4, a_5; a_6)$$

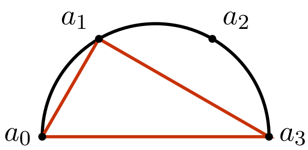
corresponds to the polygon with vertices $\{a_0, a_1, a_3, a_6\}$:

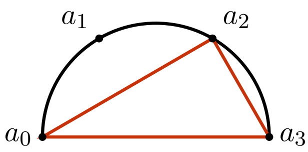


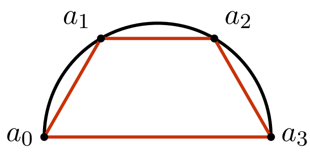
This gives us a very powerful and visual way of obtaining the coproduct of motivic iterated integrals. To be crystal clear: for each term of the sum, the term on the LHS of the tensor product has the vertices of the (red) polygon as entries, while the 'product' term on the RHS has the vertices of the (black) sub-polygons as entries. This is a one-to-one correspondence, so each polygon produces a term of the sum. Looking at all the possible polygons gives us the coproduct.

Example 5.3.5. For $n = 2$, the possible polygons with endpoints at a_0 and a_3 are as follows:









By Goncharov's theorem (respecting the order of polygons above), this give us the coproduct:

$$\begin{aligned}\Delta I^{\mathfrak{m}}(a_0; a_1, a_2; a_3) = 1 \otimes I^{\mathfrak{m}}(a_0; a_1, a_2; a_3) + I^{\mathfrak{m}}(a_0; a_1; a_3) \otimes I^{\mathfrak{m}}(a_0; a_1) I^{\mathfrak{m}}(a_1; a_2; a_3) \\ + I^{\mathfrak{m}}(a_0; a_2; a_3) \otimes I^{\mathfrak{m}}(a_0; a_1; a_2) I^{\mathfrak{m}}(a_2; a_3) + I^{\mathfrak{m}}(a_0; a_1, a_2; a_3) \otimes 1 \,.\end{aligned}$$

Remark 5.3.6. The fact that this coproduct is indeed compatible with its associated product $ш$, as it should in a Hopf algebra, is not at all obvious from Goncharov's formula. We illustrate compatibility for the example above, but note that it holds *by definition* of a coproduct. The details of how this coproduct arises at all will not be discussed, relying on substantial theory which can be found in [BGF, Chapter 5].

We use notation which is reminiscent of the harmonic algebra. Recall that for $a_0 = 0, a_{n+1} = 1$ and all $a_i \in \{0, 1\}$, motivic iterated integrals correspond to motivic MZVs. For example,

$$I^{\mathfrak{m}}(0; 0, 1; 1) = \zeta^{\mathfrak{m}}(2) \,,$$

which we can write as $z_2 = xy$. Although divergent, we mirror the binary form as usual and write

$$I^{\mathfrak{m}}(0; 0; 1) = x, \qquad I^{\mathfrak{m}}(0; 0, 1; 1) = y, \qquad I^{\mathfrak{m}}(0; 1, 0; 1) = yx \qquad \text{etc.}$$

It follows that

$$\begin{aligned}\Delta(xy) &= \Delta(I^{\mathfrak{m}}(0; 0, 1; 1)) \\ &= I^{\mathfrak{m}}(0; 0, 1; 1) \otimes 1 + I^{\mathfrak{m}}(0; 0; 1) \otimes I^{\mathfrak{m}}(0; 1; 1) + I^{\mathfrak{m}}(0; 1; 1) \otimes I^{\mathfrak{m}}(0; 0; 1) + 1 \otimes I^{\mathfrak{m}}(0; 0, 1; 1) \\ &= xy \otimes 1 + x \otimes y + y \otimes x + 1 \otimes xy\end{aligned}$$

and

$$\begin{aligned}\Delta(yx) &= \Delta(I^{\mathfrak{m}}(0; 1, 0; 1)) \\ &= I^{\mathfrak{m}}(0; 1, 0; 1) \otimes 1 + I^{\mathfrak{m}}(0; 1; 1) \otimes I^{\mathfrak{m}}(1; 0; 1) + I^{\mathfrak{m}}(0; 0; 1) \otimes I^{\mathfrak{m}}(0; 1; 0) + 1 \otimes I^{\mathfrak{m}}(0; 1, 0; 1) \\ &= yx \otimes 1 + 1 \otimes yx \,.\end{aligned}$$

Summing up, we obtain

$$\begin{aligned}\Delta(x ш y) &= \Delta(xy + yx) \\ &= (xy + yx) \otimes 1 + x \otimes y + y \otimes x + 1 \otimes (xy + yx) \\ &= (x ш y) \otimes 1 + x \otimes y + y \otimes x + 1 \otimes (x ш y) \\ &= (x \otimes 1 + 1 \otimes x) ш (y \otimes 1 + 1 \otimes y) \\ &= \Delta(x) ш \Delta(y) \,,\end{aligned}$$

where we note that $(a \otimes b) ш (c \otimes d) := (a ш c) \otimes (b ш d)$. Thus we obtain the compatibility requirement of a bialgebra $(\mathcal{H}, ш, \Delta)$ for this specific example, namely

$$\Delta(x ш y) = \Delta(x) ш \Delta(y) \,.$$

Before moving on, we state the following proposition and give a proof. We have found neither the statement nor the proof in others' work, although it seems to be implicitly acknowledged.

Proposition 5.3.7. The coproduct respects weight, in the following sense. For a motivic iterated integral

$$I = I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) \in \mathcal{H}\,,$$

we define its weight to be n (which agrees with MZVs). For a product *or* tensor product of two such integrals I_1, I_2 with weights n_1, n_2, we define its weight to be $n_1 + n_2$ (again agreeing since the product of MZVs adds their weights). Then the claim is that each summed terms in the coproduct $\Delta(I)$ has weight $n = wt(I)$, so we can write

$$wt(\Delta(I)) = wt(I)\,.$$

Equivalently, define $\mathcal{H}_n$ the subspace of $\mathcal{H}$ of elements of weight n, and write

$$\Delta(\mathcal{H}_n) \subset \mathcal{H}_n\,.$$

Proof. In Appendix A.5. □

After having introduced this coproduct, Goncharov rightly asks the question: "why do we care about motivic iterated integrals"? The answers are manifold, and its consequences may be unclear for the reader, but some of them are reproduced in my own words as follows:

1. Unlike numbers, motivic iterated integrals form a Hopf algebra.
2. The transcendental aspect of MZVs (namely, whether MZVs such as $\zeta(2k+1)$ are transcendent and algebraically independent) is eliminated. For example, it is entirely out of reach whether MZVs are linearly independent over $\mathbb{Q}$, say whether $\zeta(5) \notin \mathbb{Q}$. However, Goncharov claims that it is easy to show that the motivic elements $\zeta^{\mathfrak{m}}(2k+1)$ are linearly independent over $\mathbb{Q}$, so the motivic objects are well-understood.
3. To show that linear independence of $\zeta^{\mathfrak{m}}(2k+1)$ implies linear independence of $\zeta(2k+1)$, one needs to show that all relations among MZVs have motivic origin, i.e. come from relations among motivic MZVs to which we apply the period map. This is expected to hold, encapsulated in the conjecture [Gon, Conjecture 1.3] that the period map per is injective, and therefore an isomorphism.

This gives good reasons to study the motivic versions of MZVs, and has proven very quickly to be powerful. Before stating Brown's Theorem as the strongest of examples, we attempt to give an insight into the particular relevance of Goncharov's coproduct. It is beyond our reach to explain why it is fundamental to Brown (and others') results, but we give a few indications and an application to Higgs boson amplitudes in the next section.

5.4 The decomposition algorithm

The essential idea of this section is that the coproduct allows us to use information about MZVs strictly below a given weight n to answer questions, construct relations or decompose MZVs in weight n. In particular, we introduce an idea with applications in physics, and give a simplified version of the decomposition algorithm.

We have proved that the coproduct preserves weight, but the idea is to look at each side of the tensor product separately. We then see that all such components have strictly lower weight *except* for the cases $k = 0$ and $k = n$, which give exactly the terms

$$I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) \otimes 1 \qquad \text{and} \qquad 1 \otimes I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1})$$

respectively. We call these the *identity* terms, corresponding to the full and empty polygons. Removing these by defining the *reduced* coproduct

$$\Delta' = \Delta - \mathrm{id} \otimes 1 - 1 \otimes \mathrm{id}\,,$$

we conclude that all components of terms in Δ' have weight strictly lower than n. We give our own proof as follows. Recall that Goncharov's theorem states

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

where $0 \leq k \leq n$. The cases $k = 0$ and $k = n$ correspond exactly to the 'identity terms' above, so Δ' acts with exactly the same formula, but restricted to $1 \leq k \leq n-1$. Now $k \leq n-1$ insures that the left component

$$I^{\mathfrak{m}}(a_0; a_{i_1}, \ldots, a_{i_k}; a_{n+1})$$

has weight strictly less than n. On the other hand, $k \geq 1$ insures that the product

$$\prod_{p=0}^{k} I^{\mathfrak{m}}(a_{i_p}; a_{i_p+1}, \ldots, a_{i_{p+1}-1}; a_{i_{p+1}})$$

has weight strictly less than n, since its weight is

$$\sum_{p=0}^{k} i_{p+1} - i_p - 1 = i_{k+1} - i_0 - (k+1) = n - k\,.$$

We conclude that each side of the tensor product has weight strictly less than n.

Definition 5.4.1. We call $a \in \mathcal{H}$ a *primitive* element if $\Delta'(a) = 0$, and denote the set of primitive elements by $\mathcal{H}'$.

Note that Δ' is linear because both coproduct and tensor product are, so $\mathcal{H}'$ is a $\mathbb{Q}$-vector space. Now comes the crucial remark. If we take $a, b \in \mathcal{H}$ of weight n and find that

$$\Delta'(a) = \Delta'(b)\,,$$

then we can conclude by linearity that $a - b$ is a primitive element. In other words,

$$a = b + p$$

for some $p \in \mathcal{H}'$. This may not seem like much, but $\mathcal{H}'$ turns out to be very small when restricted to the subspace $\mathcal{M}$ of motivic MZVs. The following theorem makes this precise, which I have not seen explicitly anywhere but seems to be assumed in [Bro2].

Theorem 5.4.2. Let $\mathcal{M}' \subset \mathcal{H}'$ the space of primitive MZV elements. Then

$$\mathcal{M}' = \text{span}_{\mathbb{Q}}\{\zeta^{\mathfrak{m}}(n) \mid n \in \mathbb{N}\}\,.$$

This immediately implies that the space of primitive MZV elements of weight n is

$$\mathcal{M}'_n = \{c\zeta^{\mathfrak{m}}(n) \mid c \in \mathbb{Q}\}\,,$$

which is an extremely small (one-dimensional) space. We prove half of this theorem further down, as it requires relations which are better stated once the main idea is clear.

Coming back to our scenario, assume that we find $a, b \in \mathcal{M}$ of weight n satisfying

$$\Delta'(a) = \Delta'(b)\,.$$

It then follows that $\Delta'(a - b) = 0$, so $a - b \in \mathcal{M}$ is primitive and we obtain

$$a = b + c\zeta(n)$$

for some constant $c \in \mathbb{Q}$.

The crucial point is that determining whether $\Delta'(a) = \Delta'(b)$ involves using relations of weight strictly less than n only, since both sides of the tensor product are of lower weight. It follows that knowing relations in lower weight provides us with relations in weight n! Of course, c remains unknown and this fact does not seem to help at first sight. However, it turns out that c can be found by numerical approximation methods to arbitrarily high certainty. Indeed, a fun result to prove is that a number is rational (if and) only if its decimal expansion contains a periodic sequence of digits. Then computing many digits of

$$c = \frac{a - b}{\zeta^{\mathfrak{m}}(n)} \in \mathbb{Q}$$

will eventually give us a recurring sequence, which can be associated to a unique rational number. Of course, it could be that we computed too few digits and identified the wrong period, so the result is not exact. But computing more and more digits (which can easily be done with *very* high precision) can provide us with a satisfactory degree of certainty. Brown "hope[s] that one can give a theoretical upper bound for the prime powers which can occur in the denominators [of c] as a function of the weight (and choice of basis)" [Bro2, p.16]. If this is the case, then we can hope that c has a relatively 'nice' denominator, i.e. a relatively short periodic sequence in its decimal expansion.

As a consequence, we obtain a new relation $a = b + c\zeta^{\mathfrak{m}}(n)$ from relations of strictly lower weight. After taking the period map, this gives us a new, inductive way to construct relations among MZVs. This came as a striking surprise to me: the (expected) grading of MZVs by weight does not *a priori* suggest any 'interaction' between different layers. We provide our own examples of this method and their application in physics further on, but require some relations among motivic MZVs which will immensely simplify coproduct calculations.

The following are provided in [Bro2, Sec 5.1]. In practice, the reader who wishes to use motivic MZVs without having to learn the underlying theory should take them as a black box, and see what they can obtain. Note that Brown uses a 'reversed' notation for MZVs in the reference, so we reformulate them so as to stick with our usual notation.

Proposition 5.4.3. For all $a_i \in \{0,1\}$, the motivic elements $I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1})$ satisfy the following relations.

R0: For $n_i \geq 2$, $n_r \geq 2$,

$$I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n_1}, \ldots, \underbrace{0, \ldots, 0, 1}_{n_r}; 1) = (-1)^r \zeta^{\mathfrak{m}}(n_1, \ldots, n_r)\,.$$

R1: For $n \geq 1$, $I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) = 0$ if $a_0 = a_{n+1}$ or $a_1 = \ldots = a_n$.

R2: $I^{\mathfrak{m}}(a_0; a_1; a_2) = 0$ and $I^{\mathfrak{m}}(a_0; a_1) = 1$.

R3: $I^{\mathfrak{m}}(0; a_1, \ldots, a_n; 1) = (-1)^n I^{\mathfrak{m}}(1; a_n, \ldots, a_1; 0)$.

R4: $I^{\mathfrak{m}}(0; a_1, \ldots, a_n; 1) = I^{\mathfrak{m}}(0; 1 - a_n, \ldots, 1 - a_1; 1)$.

R5: For $k, n_1, \ldots, n_r \geq 1$,

$$(-1)^k I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n_1}, \ldots, \underbrace{0, \ldots, 0, 1}_{n_r}, \underbrace{0, \ldots, 0}_{k}; 1)$$
$$= \sum_{i_1 + \ldots + i_r = k} \binom{n_1 + i_1 - 1}{i_1} \cdots \binom{n_r + i_r - 1}{i_r} I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n_1 + i_1}, \ldots, \underbrace{0, \ldots, 0, 1}_{n_r + i_r}; 1)\,.$$

Note that taking the period map gives us the corresponding relations among MZVs.

Proof. In Appendix A.5 except **R3**, for which we refer to [Gon, Proposition 2.1]. □

With these in hand, we can proceed to proving half of Theorem 5.4.2. All we need is the following Lemma, stated in [Bro2] without proof. We give our own in Appendix A.5.

Lemma 5.4.4. For any $n \in \mathbb{N}$,

$$\Delta\zeta(n) = \zeta(n) \otimes 1 + 1 \otimes \zeta(n)\,.$$

This lemma implies half of the theorem's proof. Namely,

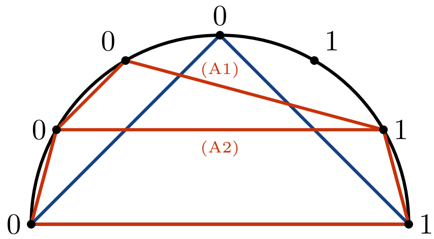
$$\Delta'(\zeta(m)) = \zeta(n) \otimes 1 + 1 \otimes \zeta(n) - \zeta(n) \otimes 1 - 1 \otimes \zeta(n) = 0\,,$$

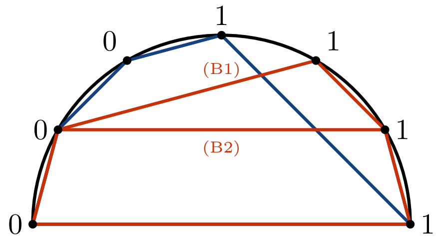
so any linear combination of such elements is primitive by linearity. In other words,

$$\mathcal{M}' \supset \operatorname{span}_{\mathbb{Q}}\{\zeta^{\mathfrak{m}}(n) \mid n \in \mathbb{N}\}\,.$$

Proving the other half is too difficult with our current formulation of the coproduct. One way around this is to use an 'infinitesimal' version of the coproduct, which simplifies its formula. This also leads to Brown's *decomposition algorithm*, but is a little technical for the purposes of this report. My aim is to appreciate the underlying idea, which we will expose in simpler (but incomplete) words after a few examples and application of the method above.

Example 5.4.5. We consider $a = I^{\mathfrak{m}}(0;0,0,0,1,1;1) = \zeta^{\mathfrak{m}}(4,1)$ and $b = (0;0,0,1,1,1;1) = \zeta^{\mathfrak{m}}(3,1,1)$ in weight $\mathcal{M}_5$. Relations **R1-R2** send most terms (polygons) of Goncharov's coproduct to 0, and in this case only two terms are non-vanishing except for the identity ones (full and empty polygons). We mark these in red below, with the blue polygons given as examples of vanishing terms.





The blue terms vanish for the following reasons. The first one vanishes because the LHS of Goncharov's formula is $I^{\mathfrak{m}}(0;0;1)$, which is zero by relation **R2**. The second one vanishes because the RHS contains the (last sub-polygon) term $I^{\mathfrak{m}}(1;1,1;1)$, which is zero by relation **R1**.

Using relations **R0-R2**, the terms (A1) and (A2) correspond to

$$I^{\mathfrak{m}}(0;0,0,1;1) \otimes I^{\mathfrak{m}}(0;0)I^{\mathfrak{m}}(0,0)I^{\mathfrak{m}}(0;0,1;1)I^{\mathfrak{m}}(1;1) = -\zeta^{\mathfrak{m}}(3) \otimes \zeta^{\mathfrak{m}}(2)$$

and

$$I^{\mathfrak{m}}(0;0,1;1) \otimes I^{\mathfrak{m}}(0;0)I^{\mathfrak{m}}(0;0,0,1;1)I^{\mathfrak{m}}(1;1) = -\zeta^{\mathfrak{m}}(2) \otimes \zeta^{\mathfrak{m}}(3)$$

respectively. Similarly, the terms (B1) and (B2) correspond to

$$I^{\mathfrak{m}}(0;0,1,1;1) \otimes I^{\mathfrak{m}}(0;0)I^{\mathfrak{m}}(0;0,1;1)I^{\mathfrak{m}}(1;1)I^{\mathfrak{m}}(1;1) = -\zeta^{\mathfrak{m}}(2,1) \otimes \zeta^{\mathfrak{m}}(2)$$

and

$$I^{\mathfrak{m}}(0;0,1;1) \otimes I^{\mathfrak{m}}(0;0)I^{\mathfrak{m}}(0;0,1,1;1)I^{\mathfrak{m}}(1;1) = -\zeta^{\mathfrak{m}}(2) \otimes \zeta^{\mathfrak{m}}(2,1)$$

respectively. Since the reduced coproduct kills the identity terms, we obtain

$$\Delta'(a) = -\zeta^{\mathfrak{m}}(3) \otimes \zeta^{\mathfrak{m}}(2) - \zeta^{\mathfrak{m}}(2) \otimes \zeta^{\mathfrak{m}}(3)$$

and

$$\Delta'(b) = -\zeta^{\mathfrak{m}}(2,1) \otimes \zeta^{\mathfrak{m}}(2) - \zeta^{\mathfrak{m}}(2) \otimes \zeta^{\mathfrak{m}}(2,1)\,.$$

Now we asumme that we have proceeded with this procedure by induction on weight, and in particular we would easily have obtained the motivic version of Euler's identity

$$\zeta^{\mathfrak{m}}(2,1) = \zeta^{\mathfrak{m}}(3)\,.$$

by calculating their respective coproducts. Alternatively, this is immediately given by the duality relation **R4**. As a result, we obtain

$$\Delta'(a) = \Delta'(b)$$

and thus, $a - b$ is a primitive element. Now Theorem 5.4.2 implies that

$$a = b + c\zeta^{\mathfrak{m}}(5)$$

for some rational c. Using PARI/GP we obtain the evaluation

$$\frac{a-b}{\zeta^{\mathfrak{m}}(5)} = 0.0000\ldots$$

with $1,000$ digit precision, which implies the relation

$$a = b$$
$$\zeta^{\mathfrak{m}}(4,1) = \zeta^{\mathfrak{m}}(3,1,1)$$

with very high certainty. The crucial point here is that we were able to deduce this relation in weight 5 from a relation of lower weight 3, which is not obvious at all!

Application. The method I have given above has been applied to Higgs boson amplitudes by Claude Duhr in his paper [Duh]. He uses the coproduct directly (rather than the infinitesimal version given further down), descending into as many tensor products as necessary.

As previously mentioned, multiple zeta values arise naturally in quantum field theory, as terms coming from Feynman diagrams. Other terms arise including multiple polylogarithms (MPs), and it turns out that these can also be written as iterated integrals. As such, Duhr observed that the Hopf algebra structure $\mathcal{H}$ we have introduced could be used in simplifying complicated expressions for "multi-loop amplitudes in perturbative quantum field theory". This is significant because MPs "are assumed to cover large classes of phenomelogically interesting Feynman integrals" (p.2).

One approach to deal with MPs was a so-called symbol-based approach, but highly valuable information was lost in the process because all MZVs are sent to zero by the symbol. On the contrary, the coproduct preserves information about most MZVs, the only exception being single zetas $\zeta(m)$. Duhr noticed this and applied Goncharov and Brown's work to upgrade the symbol-based approach and improve it significantly. In slightly different language, he considers a function F_w of weight w and assumes that we can find a simpler function G_w such that

$$\Delta'(F_w) = \Delta'(G_w)\,.$$

He then writes that we must have

$$F_w = G_w + \sum_i c_i P_{w,i}$$

for some primitive elements $P_{w,i} \in \mathcal{H}$ and $c_i \in \mathbb{Q}$. In the case of MZVs, the primitive elements were only the single zetas, but here we have a slightly larger class. The primitive elements are powers of π (which is partially the case for us, since $\zeta(2n)$ is a power of π), single zetas $\zeta(n)$, and "Clausen values at the roots of unity",

$$Cl_n\left(\frac{k\pi}{N}\right) = \mathfrak{R}_n\left[\mathrm{Li}_n\left(e^{ik\pi/N}\right)\right]$$

where $\mathfrak{R}_n$ is the real part for n even and imaginary part for n odd. This is not much more complicated than what we obtained for motivic MZVs only, and undoubtedly improves on the symbol approach. Following Duhr, we give an example for polylogarithms at the special value $x = 1/2$, as follows. We do not work through the calculations in detail, but they really do stem from Goncharov's formula and the expression of MPs as iterated integrals in $\mathrm{per}(\mathcal{H})$. Note that $\mathrm{Li}_n(x)$ is precisely what we call polylogarithms, and the multi-variate case $\mathrm{Li}_{n_1,\ldots,n_s}\, x_1, \ldots, x_r$ is called a MP. From Goncharov's theorem, we apply Δ twice to obtain

$$\begin{aligned}\Delta_{1,1}\left[\mathrm{Li}_2\left(\frac{1}{2}\right)\right] &= -\ln\left(1-\frac{1}{2}\right)\otimes\ln\left(\frac{1}{2}\right)\\ &= -\ln(2)\otimes\ln(2)\\ &= -\frac{1}{2}\Delta_{1,1}(\ln^2(2)),\end{aligned}$$

noting that $-\ln\left(\frac{1}{2}\right) = \ln(2)$. Since $\zeta(2)$ is a rational multiple of π^2 and we cannot obtain a Clausen value for reasons of weight, this implies that

$$\mathrm{Li}_2\left(\frac{1}{2}\right) = -\frac{1}{2}\ln^2(2) + c\pi^2$$

for some $c \in \mathbb{Q}$. By numerical approximation performed ourself with PARI/GP, we obtain

$$c = \frac{\mathrm{Li}_2\left(\frac{1}{2}\right) + \frac{1}{2}\ln^2(2)}{\pi^2} = 0.08333333...$$

with 1000 digits 3 following it, from which we can reasonably conclude that $c = \frac{1}{12}$. Finally, we obtain the non-trivial relaton

$$\mathrm{Li}_2\left(\frac{1}{2}\right) = -\frac{1}{2}\ln^2(2) + \frac{1}{12}\pi^2.$$

This concludes the example. The method above has the caveat that one must make good choices for the elements a, b on which we act with the coproduct. A more precise, less *ad hoc* way of using the coproduct is by way of a 'decomposition' algorithm. Assume we have a set of elements $B \subset \mathcal{M}$ which we expect to be a basis, for theoretical or numerical reasons (say Hoffman's elements). Taking any $a \in \mathcal{M}$ of weight n, we would like to write a as a linear combination of elements in B. This would give us both a new relation and an explicit representation of a in this basis: something highly worth seeking. We proceed by induction, and work all the way up to writing all elements of weight $k \leq n-1$ in terms of B. First note that the base case $n = 2$ only has one element, so the claim holds as long as B_1 contains $\zeta^{\mathfrak{m}}(2)$, as it should. Now for any element a of weight n, compute

$$\Delta'(a) \qquad \text{and} \qquad \Delta'(b_i)$$

for all $b_i \in B_n$, where $B_n \subset B$ are those elements of weight n. Both sides of the tensor product of terms in $\Delta'(a)$ and $\Delta'(b)$ have weight strictly less than n, so we can write all of them in the basis B. From this, we would like to write $\Delta'(a)$ as a linear combination of $\Delta'(b_i)$. This cannot be done in general because the tensor space we are left with has much larger dimension that the elements at our disposal (only $\#B_n$). We will not describe how to resolve this in detail, but the idea is that we can eliminate one side of the tensor product by acting on it and turning it into a rational number, which we simply place in front of the other half. This will give us a space that is small enough to be re-expressed in terms of B, *provided* that our choice of B_n is indeed a basis for $\mathcal{M}_n$. Assuming this works, we obtain

$$\Delta'(a) = \sum_{i=1}^{\#B_n} c_i \Delta'(b_i)$$

and therefore

$$a = \sum_{i=1}^{\#B_n} c_i b_i + c\zeta^{\mathfrak{m}}(n)$$

for some known constants $c_i \in \mathbb{Q}$. As previously mentioned, we can find c to high numerical precision. If B contains $\zeta^{\mathfrak{m}}(n)$, we have written a in terms of B and are done. If not, Brown claims in [Bro2, p. 16] that a slight variant of (his rigorous version of) this algorithm allows us to decompose a in terms of B anyway. Thus the algorithm is successful, not only in writing all motivic MZVs in terms of B if it is a basis, but in checking whether B is indeed a basis at each weight along the way.

Even more than this, notice that all relations up to now were produced in a sporadic, unordered way. EDS, Ohno, derivation: none of these were able to generate relations which were guaranteed to involve an exact set of MZVs chosen beforehand. This is precisely why all such families, although powerful, were not able to be counted (to bound the dimension) nor led to writing a specific spanning set (a potential basis like Hoffman's family). On the contrary, this inductive decomposition allows to write *any* MZV into a linear combination of a chosen set B, as long as this set is large enough to contain a spanning set – which is not hard to pick appropriately by numerical simulation.

The inductive method described above is a purposefully rough sketch of Brown's decomposition algorithm in [Bro2]. I have done my best to give an intuition for his algorithm and the technicalities involved while making the process clear, but am aware that the description is incomplete. My aim was to give an intuitive justification of the coproduct's strength in studying MZV's, without having to re-formulate Brown's work, which involves the infinitesimal coproduct. Instead, I encourage the enthusiastic reader to explore Brown's paper for a rigorous treatment.

5.5 Brown's Theorem and consequences

Brown was inspired from Goncharov's seminal work, but took a different direction with regards to subtleties about even zetas. The major difference is that Goncharov's construction yields

$$\zeta^{\mathfrak{m}}(2k) = 0$$

for all $k \geq 1$, so the coproduct loses all information on terms proportional to π^2. This seems fine for our purposes, considering that the objects $\zeta(2k)$ have explicit formulae and may not require further understanding. On the contrary, even motivic zetas are defined differently in Brown's work, providing crucial information that was necessary to prove his main theorem.

Brown's Theorem. The set of elements

$$\{\zeta^{\mathfrak{m}}(s_1,\ldots,s_r) \mid s_i \in \{2,3\}\}$$

is a basis for the $\mathbb{Q}$-vector space of motivic multiple zeta values $\mathcal{M}$.

Remark 5.5.1. This immediately implies the version of his theorem for usual MZVs stated in Section 5.1, obtained by applying the period map. Indeed, taking any MZV $\zeta(\mathbf{a})$, we have $\mathrm{per}(\zeta^{\mathfrak{m}}(\mathbf{a})) = \zeta(\mathbf{a})$ by definition of per. Now Brown's Theorem implies that we can write this motivic MZV as a linear combination with only 2's and 3's as entries, and taking the period map gives us $\zeta(\mathbf{a})$ as a linear combination of their projections, which have exactly the same multi-index and therefore only 2's and 3's as entries!

It cannot be understated that this could not (for now) have been accomplished without the theory of motives, despite the difficulty in apprehending it for young and more experienced readers alike. The extra structure provided by the 'lift' is fundamental to Brown's result.

At this point, one should ask: if this theorem proves that (motivic) Hoffman's elements form a basis for $\mathcal{M}$, can the result be reproduced for any other choice of elements which we numerically expect to form a basis? The answer is no, because Hoffman's family have a particularly nice structure with respect to the coproduct. It turns out that the subspace $\mathcal{M}^{2,3}$ is 'stable' under the coaction, namely

$$\Delta : \mathcal{M}^{2,3} \longrightarrow \mathcal{M} \otimes \mathcal{M}^{2,3}\,.$$

The right-hand side is the only one which really matters in the infinitesimal setting, which gives us a very elegant stability property. This again suggests why the coproduct is essential. It should be said that another central component of his proof involves an identity among MZVs contributed by Zagier, which was then lifted to its motivic counterpart using the infinitesimal 'coproduct' operators.

The fact that we do not know whether all relations among MZVs have motivic origin is precisely why Brown's Theorem gives us a spanning set, but not yet a basis. If the period map is injective as conjectured, then this is indeed a basis and we are done. To conclude this section, we give a few corollaries of Brown's Theorem.

Corollary 5.5.2. Zagier's conjecture is equivalent to the period map being injective.

Proof. Brown's Theorem implies that the vector space of motivic MZVs of weight k is of dimension d_k, by the counting argument I gave in Section 5.1. Zagier's conjecture is that $\mathcal{Z}_k$ has dimension d_k, which can only hold (since per is a linear map between vector spaces) if the period map is an isomorphism (i.e. injective), and vice-versa. □

Corollary 5.5.3. Zagier's conjecture is equivalent to Gröthendieck's period conjecture for mixed Tate motives.

The result is proved in [BGF, Corollary 5.51]. Note that Gröthendieck's period conjecture is a deep and long-standing one, so it is impressive to see it crop up as being equivalent to a conjecture regarding MZVs only. This last corollary is our favourite.

Corollary 5.5.4. Zagier's conjecture implies the transcendence conjecture, namely that

$$\pi, \zeta(3), \zeta(5), \dots$$

are algebraically independent.

In particular, recall that the transcendence conjecture implies that all odd zeta values are transcendent. This lends much credit to Goncharov's visionary statement in [Gon, p. 5]: "I think that an understanding of the transcendental aspects of the iterated integrals is impossible without investigation of the corresponding motivic objects".

The proof can be found in [BGF, Corollary 5.49], although requires some understanding of the underlying motivic theory. It also relies on a theorem by Milor-Moore on Hopf algebras, which essentially allows us to linearise the question. More precisely, the theorem allows us to obtain algebraic indepence from the linear independence of motivic odd zetas, which is guaranteed by the theory.

I hope that this chapter helped the reader to appreciate how and why this theory has proven to be powerful in the study of MZVs, despite the healthy amount of hand-waving involved. It is meant only as a flavour to start with rather than a detailed exploration, for which we would again recommend BGF.

To conclude this report, I would like to give a short list of personal, sketch ideas that I hope are interesting and reasonable. I would very much have liked to spend more time on pursuing them.

1. A construction of motivic t-MZVs. The interesting variants in structure that t-MZVs manifest may well have interesting consequences when lifted to their motivic counterparts, in particular at $t = 1/2$ and $t = 1$. On the other hand, this may well not yield anything of interest. The integral formulation of MZVs looks by far to be the cleanest among t-zetas (recall that duality did not transpose well for any other t), and the entire theory is based on iterated integrals as opposed to sums. Half-zetas have particularly nice stuffle and other features because of their sum formulation, so this is possibly a red herring. Regardless, the first step in this direction is to construct a more general coproduct Δ^t which is compatible with the t-shuffle product. It seems as though we can simply take $\Delta^t = \Delta$ to obtain

$$\begin{aligned}\Delta^t(\zeta^t(a)\zeta^t(b)) &= \Delta(Z \circ S^t(a \overset{t}{\sqcup\!\sqcup} b))) \\ &= \Delta(Z \circ S^t(a) \sqcup\!\sqcup Z \circ S^t(b)) \\ &= \Delta(Z \circ S^t(a)) \sqcup\!\sqcup \Delta(Z \circ S^t(b)) \\ &= \Delta^t(\zeta^t(a))\Delta^t(\zeta^t(b))\end{aligned}$$

as required, which can easily be made more formal using the harmonic algebra (in particular making the t-shuffle product $\overset{t}{\sqcup\!\sqcup}$ appear explicitly at the end, instead of hiding it as a product). The issue that arises in using this coproduct is that we would like computations of the coproduct to be 'closed', in the sense that computing $\Delta^t(\zeta^t(a))$ should give us an answer involving tensor products of t-zetas directly. The above formulation gives no indication as to how to do this efficiently, since it involves decomposing into usual zetas through the operator S^t, and taking the inverse afterwards. More precisely, we would like to involve Goncharov's formula in such a way as to obtain

$$\Delta^t(\zeta^t(a)) = h^t(\Delta(\zeta(a)))$$

for some function h^t dependent on t, as for S^t.

2. An analytic continuation of multiple zeta functions is provided in [Zha], and it would be interesting to see whether similar algebraic structure is exhibited among other values than the positive integers. In particular, it may be worthwhile to look into the space of multiple zeta functions evaluated at $(a_1+i, \dots, a_r+i)$ where a_j are positive integers with $a_1 \geq 2$, as for MZVs but with $i \in \mathbb{C}$ added in every slot. The choice of i rather than any other integer multiple of i is arbitrary, but perhaps there exist relations among such values, either uniformly in the integers plus i, or travelling across the lattice with each index in $\mathbb{N}[i]$ except for the first one, which must have real coefficient greater than 1 for convergence.

3. A probabilistic outlook on the space of MZVs as the weight k goes to infinity. Although the usefulness of such a question is doubtful, I have always found these questions interesting in themselves and worthwhile to pursue. My question goes as follows.

Question: Let p_k the probability that a randomly generated set of d_k elements in $\mathcal{Z}_k$ forms a basis for $\mathcal{Z}_k$. Is p_k convergent? If so, what does it converge to?

Unfortunately I did not have time to complete my code for a program in PARI/GP, aimed to determine p_k by way of numerical simulation. This would only have been computationally feasible for low weight regardless, since it involves looking at all possible sets of d_k elements among 2^{k-2}, the number of which grows incredibly fast. It would still have been interesting to determine up to weight 15, although is insufficient ground to formulate a conjectural answer to this question, since the claim concerns behaviour at *extremely large* k. On the other hand, I have attended talks and read some papers on probabilistic group theory including Martin Liebeck's work, and the answer that $p_k \to 1$ as $k \to \infty$ does not sound implausible to me.

Chapter 6

Conclusion

In this report, our aim was to introduce the intricate and elusive structure living behind multiple zeta values. The first three chapters gave a detailed insight into relations among MZVs; the formal algebraic lens through which they can be studied; large families which are expected to produce everything through both algebraic and analytic procedures. We enlarged our perspective in Chapter 4, building on Yamamoto's interpolation and developing a more comprehensive generalisation of results to t-MZVs, with applications and further potential work. The major limitation of these chapters is that they give little insight into how we can use relations to construct a spanning set for MZVs. As such, we provided the basic elements to a more sophisticated and recent approach. This involved the introduction of periods, in both the naïve and cohomological sense, of which MZVs are special cases. These numbers contain information of a geometric nature, which can be lifted to a more abstract 'motivic' setting. Such objects form a Hopf algebra, satisfy certain relations and can be manipulated using Goncharov's formula for the accompanying coproduct. The decomposition algorithm is sketched and gives a way to decompose MZVs into any conjectural spanning set. The final section states Brown's impressive theorem, a few corollaries and further horizons to explore.

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Declaration

This piece of work is a result of my own work except where it forms an assessment based on group project work. In the case of a group project, the work has been prepared in collaboration with other members of the group. Material from the work of others not involved in the project has been acknowledged and quotations and paraphrases suitably indicated.

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Appendices

Appendix A

Long proofs

Long proofs are placed in this appendix, preceded by the result and a star ($\star$) linking to the statement as first introduced in the report.

A.1 Chapter 1

Theorem. ($\star$) There are infinitely many primes.

Proof. By decomposition of natural numbers into primes, any $m \in \mathbb{N}$ can be written as

$$m = p_1^{m_1} \dots p_r^{m_r}$$

with p_i primes and m_i natural numbers. This decomposition is unique and corresponds to exactly one integer m. Then a sum over *all* integers n can be rewritten as a sum over *all* products of prime powers. Thus the Riemann zeta function can be written as

$$\begin{aligned}
\zeta(s) &= \sum_{n=1}^{\infty} n^{-s} \\
&= \prod_{p \text{ prime}} \sum_{k=0}^{\infty} p^{-sk} \\
&= \prod_{p \text{ prime}} \frac{1}{1-p^{-s}} .
\end{aligned}$$

Assume that there are finitely many primes. Then the RHS is a finite product, so its evaluation at $s = 1$ is a finite number. But the LHS is the harmonic series

$$\sum_{n=1}^{\infty} \frac{1}{n} = \infty$$

which diverges. [This is widely known and can be proved by various means, but we hope the reader knows this from a first course in analysis]. This contradicts the assumption, so there are infinitely many primes. $\square$

Lemma 1.3.3. ($\star$) For any $k \geq 4$ and $2 \leq j \leq k-2$ we have

$$\zeta(j, k-j) + \zeta(k-j, j) + \zeta(k) = \sum_{r=2}^{k-1} \left[\binom{r-1}{j-1} + \binom{r-1}{k-j-1} \right] \zeta(r, k-r) \,.$$

Proof. For integers $i, j \geq 1$, we use the decomposition

$$\frac{1}{n^i m^j} = \sum_{r=1}^{i+j-1} \left[\frac{\binom{r-1}{i-1}}{(n+m)^r m^{i+j-r}} + \frac{\binom{r-1}{j-1}}{(n+m)^r n^{i+j-r}} \right]$$

whose proof can be found in [BGF, Lemma 1.31] by induction on i and j and a simple partial fraction expansion. Taking $i = k-j$ with $2 \leq j \leq k-2$ gives the first term of the RHS ($r = 1$) to be

$$\left[\frac{\binom{0}{k-j-1}}{(n+m)m^{k-1}} + \frac{\binom{0}{j-1}}{(n+m)^1 n^{k-1}} \right] = 0$$

since $j - 1 \geq 1 > 0$ and $k - j - 1 \geq 1 > 0$. Taking $k \geq 4$, this implies

$$\begin{aligned}
\zeta(k-j)\zeta(j) &= \sum_{n>0} \frac{1}{n^{k-j}} \sum_{m>0} \frac{1}{m^j} \\
&= \sum_{n>0,\, m>0} \frac{1}{n^{k-j} m^j} \\
&= \sum_{n>0,\, m>0} \sum_{r=2}^{k-1} \left[\frac{\binom{r-1}{k-j-1}}{(n+m)^r m^{k-r}} + \frac{\binom{r-1}{j-1}}{(n+m)^r n^{k-r}} \right] \\
&= \sum_{r=2}^{k-1} \left[\binom{r-1}{j-1} + \binom{r-1}{k-j-1} \right] \sum_{n>0,\, m>0} \frac{1}{(n+m)^r m^{k-r}} \,,
\end{aligned}$$

using the symmetry in interchanging $n \leftrightarrow m$, and where the change of sum order is justified by absolute convergence for $k \geq 4$ and $2 \leq r \leq k-1$. Taking $l = n + m$, we obtain

$$\begin{aligned}
\zeta(k-j)\zeta(j) &= \sum_{r=2}^{k-1} \left[\binom{r-1}{j-1} + \binom{r-1}{k-j-1} \right] \sum_{l>m>0} \frac{1}{l^r m^{k-r}} \\
&= \sum_{r=2}^{k-1} \left[\binom{r-1}{j-1} + \binom{r-1}{k-j-1} \right] \zeta(r, k-r) \,,
\end{aligned}$$

which is the RHS of the lemma. Finally, we decompose the sum

$$\zeta(k-j)\zeta(j) = \sum_{n>0,\, m>0} \frac{1}{n^{k-j} m^j}$$

into the disjoing cases $n > m$, $n < m$ and $n = m$, giving us

$$\begin{aligned}
\zeta(k-j)\zeta(j) &= \left(\sum_{n>m>0} + \sum_{m>n>0} + \sum_{n=m>0} \right) \frac{1}{n^{k-j} m^j} \\
&= \zeta(k-j, j) + \zeta(j, k-j) + \zeta(k) \,,
\end{aligned}$$

which is the LHS and concludes the proof. $\square$

Lemma 1.3.5. ($\star$) Assuming Euler's sum theorem, we have

$$T_k(X,Y) + T_k(Y,X) + \zeta(k)\frac{X^{k-1}-Y^{k-1}}{X-Y} = T_k(X+Y,Y) + T_k(X+Y,X)$$

for all $k \geq 4$.

Proof. Multiply both sides of equation ($\dagger$) by $X^{j-1}Y^{k-j-1}$ and sum over j between 2 and $k-2$. Then the LHS becomes

$$\text{LHS} = \sum_{j=2}^{k-2}\zeta(j,k-j)X^{j-1}Y^{k-j-1} + \sum_{j=2}^{k-2}\zeta(k-j,j)Y^{k-j-1}X^{j-1} + \zeta(k)\sum_{j=2}^{k-2}X^{j-1}Y^{k-j-1}\,.$$

To compensate for the missing terms (differing from the formal setting of GKZ), we add $(\zeta(k) + \zeta(k-1,1))(X^{k-2}+Y^{k-2})$ on both sides. This gives

$$\begin{aligned}\text{LHS} &= \sum_{j=2}^{k-1}\zeta(j,k-j)X^{j-1}Y^{k-j-1} + \sum_{j=1}^{k-2}\zeta(k-j,j)Y^{k-j-1}X^{j-1} + \zeta(k)\sum_{j=1}^{k-1}X^{j-1}Y^{k-j-1} \\ &= T_k(X,Y) + T_k(Y,X) + \zeta(k)\frac{X^{k-1}-Y^{k-1}}{X-Y}\end{aligned}$$

as required. On the other hand, the RHS becomes

$$\text{RHS} = \sum_{r=2}^{k-1}\sum_{j=2}^{k-2}\left[\binom{r-1}{j-1} + \binom{r-1}{k-j-1}\right]\zeta(r,k-r)X^{j-1}Y^{k-j-1} + (\zeta(k)+\zeta(k-1,1))(X^{k-2}+Y^{k-2})\,.$$

Assuming Euler's sum formula (!), the compensating (rightmost) term expands as

$$\begin{aligned}&(\zeta(k)+\zeta(k-1,1))(X^{k-2}+Y^{k-2}) \\ &\qquad = \sum_{r=2}^{k-1}\zeta(r,k-r)(X^{k-2}+Y^{k-2}) + \zeta(k-1,1)(X^{k-2}+Y^{k-2})\,.\end{aligned}$$

Noticing that $\binom{r-1}{k-2}$ is only non-zero when $r = k-1$, this gives us

$$\begin{aligned}&(\zeta(k)+\zeta(k-1,1))(X^{k-2}+Y^{k-2}) \\ &\qquad = \sum_{r=2}^{k-1}\left[\binom{r-1}{k-2}+1\right]X^{k-2}\zeta(r,k-r) + \sum_{r=2}^{k-1}\left[1+\binom{r-1}{k-2}\right]Y^{k-2}\zeta(r,k-r)\,.\end{aligned}$$

This corresponds exactly to the terms $j=1$ and $j=k-1$ in the leftmost term of the RHS, so we can bring them together to obtain

$$\text{RHS} = \sum_{r=2}^{k-1}\sum_{j=1}^{k-1}\left[\binom{r-1}{j-1} + \binom{r-1}{k-j-1}\right]\zeta(r,k-r)X^{j-1}Y^{k-j-1}\,.$$

It remains only to notice that this is really a binomial expansion. Firstly, note that

$$
\begin{aligned}
(X+Y)^{r-1} &= \sum_{j=0}^{r-1} \binom{r-1}{j} X^j Y^{r-1-j} \\
&= \sum_{j=1}^{r} \binom{r-1}{j-1} X^{j-1} Y^{r-j} .
\end{aligned}
$$

For $j > r$ we have $\binom{r-1}{j-1} = 0$ by definition, so for $r \leq k-1$ we can add empty terms and multiply by Y^{k-r-1} to give

$$
\begin{aligned}
(X+Y)^{r-1} Y^{k-r-1} &= \sum_{j=1}^{k-1} \binom{r-1}{j-1} X^{j-1} Y^{r-j} Y^{k-r-1} \\
&= \sum_{j=1}^{k-1} \binom{r-1}{j-1} X^{j-1} Y^{k-j-1} .
\end{aligned}
$$

By swapping X and Y and making the change of variables $j \mapsto k-j$, we similarly obtain

$$
(X+Y)^{r-1} X^{k-r-1} = \sum_{j=1}^{k-1} \binom{r-1}{k-j-1} X^{j-1} Y^{k-j-1} .
$$

Finally, the RHS becomes

$$
\begin{aligned}
\text{RHS} &= \sum_{r=2}^{k-1} \sum_{j=1}^{k-1} \left[\binom{r-1}{j-1} + \binom{r-1}{k-j-1} \right] \zeta(r, k-r) X^{j-1} Y^{k-j-1} \\
&= \sum_{r=2}^{k-1} \left[(X+Y)^{r-1} Y^{k-r-1} + (X+Y)^{r-1} X^{k-r-1} \right] \zeta(r, k-r) \\
&= T_k(X+Y, Y) + T_k(X+Y, X)
\end{aligned}
$$

which concludes the proof. □

Proposition 1.4.6. ($\star$) For $k \geq 2$, the number of admissible multi-indices of weight k is 2^{k-2}.

Proof. The number of admissible multi-indices of weight k is the number of solutions to the equation

$$
k = a_1 + \ldots + a_n
$$

with $n \geq 1$, $a_1 \geq 2$ and $a_1, \ldots, a_n$ positive integers. Let c_k be the number of such solutions, with $c_0 = c_1 = 0$. For $k \geq 2$, the possibilities for a_1 are $2, \ldots, k$. If $a_1 = k$ we must have $n = 1$, which provides us with one solution. Otherwise, choosing $a_1 \leq k-1$ gives us

$$
k - a_1 + 1 = (a_2 + 1) + a_3 + \ldots + a_n ,
$$

which has c_{k-a_1+1} solutions by definition, noting that $a_2 + 1 \geq 2$. Summing over choices of a_1 we obtain

$$
c_k = c_{k-1} + \ldots + c_2 + 1 .
$$

We now prove the statement by induction. For $k = 2$, the only admissible multi-index is (2), so $c_2 = 1 = 2^0$. For the induction step,

$$c_k = c_{k-1} + \ldots + c_2 + 1 = 2^{k-3} + \ldots + 1 + 1 = \frac{1 - 2^{k-2}}{1 - 2} + 1 = 2^{k-2}. \qquad \square$$

A.2 Chapter 2

Theorem 2.2.14. (⋆) The map $Z^* : (\mathfrak{h}^0, *) \longrightarrow (\mathbb{R}, \cdot)$ is a $\mathbb{Q}$-algebra homomorphism.

To prove this theorem, we first require the following lemma which we prove immediately below.

Lemma. For any $z_{a_1} w \coloneqq z_{a_1} \ldots z_{a_r} \in \mathfrak{h}^0$ and $p \geq 1$ we have the following identity:

$$Z^*_p(z_{a_1} w) = \sum_{p > n_1 > 0} \frac{1}{n_1^{a_1}} \, Z^*_{n_1}(w) \, .$$

Proof.

$$\begin{aligned} Z^*_p(z_{a_1} w) = \zeta_p(a_1, \ldots, a_r) &= \sum_{p > n_1 > \ldots > n_r > 0} \frac{1}{n_1^{a_1} \cdots n_r^{a_r}} \\ &= \sum_{p > n_1 > 0} \frac{1}{n_1^{a_1}} \sum_{n_1 > n_2 > \ldots > n_r > 0} \frac{1}{n_2^{a_2} \cdots n_r^{a_r}} \\ &= \sum_{p > n_1 > 0} \frac{1}{n_1^{a_1}} \, \zeta_{n_1}(a_2, \ldots, a_r) \\ &= \sum_{p > n_1 > 0} \frac{1}{n_1^{a_1}} \, Z^*_{n_1}(w) \, . \qquad \square \end{aligned}$$

Proof of Theorem. The statement is that $Z^*(a * b) = Z^*(a) Z^*(b)$ for any $a, b \in \mathfrak{h}^0$. We first prove that this holds for the p-truncated version of the equality, for all $p \geq 1$. If one of a or b is the identity, we have w.l.o.g. $Z^*_p(a * 1) = Z^*_p(a) = Z^*_p(a) \cdot 1 = Z^*_p(a) Z^*_p(1)$ as required.

Otherwise, write $a = z_{a_1} \ldots z_{a_r} \coloneqq z_{a_1} u$ and $b = z_{b_1} \ldots z_{b_s} \coloneqq z_{b_1} v$. As previously foreshadowed, we proceed by induction on $r + s$, noting that u and v have lengths $r - 1$ and $s - 1$ respectively. Take any $p \geq 1$. Starting with the LHS,

$$\begin{aligned} Z^*_p(a) Z^*_p(b) &= \zeta_p(a_1, \ldots, a_r) \zeta_p(b_1, \ldots, b_r) \\ &= \sum_{\substack{p > n_1 > \ldots > n_r > 0 \\ p > m_1 > \ldots > m_s > 0}} \frac{1}{n_1^{a_1} \cdots n_r^{a_r}} \, \frac{1}{m_1^{b_1} \cdots m_s^{b_s}} \\ &= \left(\sum_{\substack{p > n_1 > \ldots > n_r > 0 \\ p > n_1 > m_1 > \ldots > m_s > 0}} + \sum_{\substack{m_1 > n_1 > \ldots > n_r > 0 \\ m_1 > \ldots > m_s > 0}} + \sum_{\substack{k_1 > n_2 \ldots > n_r > 0 \\ k_1 > m_2 \ldots > m_s > 0}} \right) \frac{1}{n_1^{a_1} \cdots n_r^{a_r}} \, \frac{1}{m_1^{b_1} \cdots m_s^{b_s}} \end{aligned}$$

where the three terms come from splitting into cases $n_1 > m_1$, $n_1 < m_1$ and $n_1 = m_1 := k_1$ respectively. The first term gives us:

$$\begin{aligned}\sum_{\substack{p>n_1>\ldots>n_r>0\\ p>n_1>m_1>\ldots>m_s>0}} \frac{1}{n_1^{a_1}\cdots n_r^{a_r}}\frac{1}{m_1^{b_1}\cdots m_s^{b_s}} &= \sum_{p>n_1>0}\frac{1}{n_1^{a_1}}\sum_{\substack{n_1>n_2>\ldots>n_r>0\\ n_1>m_1>\ldots>m_s>0}}\frac{1}{n_2^{a_2}\cdots n_r^{a_r}}\frac{1}{m_1^{b_1}\cdots m_s^{b_s}}\\ &= \sum_{p>n_1>0}\frac{1}{n_1^{a_1}}\zeta_{n_1}(a_2,\ldots,a_r)\zeta_{n_1}(b_1,\ldots,b_s)\\ &= \sum_{p>n_1>0}\frac{1}{n_1^{a_1}}Z^*_{n_1}(u)Z^*_{n_1}(b)\,.\end{aligned}$$

After similar calculations for the other two terms, we use the induction step and Lemma **??** to conclude:

$$\begin{aligned}Z^*_p(a)Z^*_p(b) &= \sum_{p>n_1>0}\frac{1}{n_1^{a_1}}Z^*_{n_1}(u)Z^*_{n_1}(b) + \sum_{p>m_1>0}\frac{1}{m_1^{b_1}}Z^*_{m_1}(a)Z^*_{m_1}(v) + \sum_{p>k_1>0}\frac{1}{k_1^{a_1+b_1}}Z^*_{k_1}(u)Z^*_{k_1}(v)\\ &= \sum_{p>n_1>0}\frac{1}{n_1^{a_1}}Z^*_{n_1}(u*b) + \sum_{p>m_1>0}\frac{1}{m_1^{b_1}}Z^*_{m_1}(a*v) + \sum_{p>k_1>0}\frac{1}{k_1^{a_1+b_1}}Z^*_{k_1}(u*v)\\ &= Z^*_p(z_{a_1}(u*b)) + Z^*_p(z_{b_1}(a*v)) + Z^*_p(z_{a_1}\circ z_{b_1}(u*v))\\ &= Z^*_p(z_{a_1}(u*b) + z_{b_1}(a*v) + z_{a_1}\circ z_{b_1}(u*v))\\ &= Z^*_p(a*b)\,,\end{aligned}$$

which completes the induction. Finally, take the limit $p\to\infty$ and use Remark 2.2.17 to complete the proof:

$$\begin{aligned}\lim_{p\to\infty} Z^*_p(a)Z^*_p(b) &= \lim_{p\to\infty} Z^*_p(a*b)\\ Z^*(a)Z^*(b) &= Z^*(a*b)\,.\end{aligned}$$

□

Corollary 2.2.19. ($\star$) $(\mathcal{Z},\cdot)$ is a graded algebra.

Proof. The fact that $(\mathcal{Z},\cdot)$ is an algebra follows immediately from writing

$$\zeta(a_1,\ldots,a_r)\zeta(b_1,\ldots,b_s) = \zeta(z_{a_1}\ldots z_{a_r})\zeta(z_{b_1}\ldots z_{b_s}) = \zeta((z_{a_1}\ldots z_{a_r})*(z_{b_1}\ldots z_{b_s}))$$

for any MZVs. Now note that the stuffle product is a finite linear combination of words in $\mathfrak{h}^0$, so that the MZV product decomposes as a finite linear combination of MZVs. In other words $\cdot:\mathcal{Z}\times\mathcal{Z}\longrightarrow\mathcal{Z}$ is a binary operation on $\mathcal{Z}$, as required to make $\mathcal{Z}$ an algebra.

To show that $\mathcal{Z}$ is graded, take admissible multi-indices $\mathbf{a}=(a_1,\ldots,a_r),\mathbf{b}=(b_1,\ldots,b_s)$ of weights n,m respectively. We need to show that $\zeta(\mathbf{a})\zeta(\mathbf{b})\in\mathcal{Z}_{n+m}$. Writing $u=z_{a_1}\ldots z_{a_r}$ and $v=z_{b_1}\ldots z_{b_s}$, Theorem 2.2.14 implies that

$$\zeta(\mathbf{a})\zeta(\mathbf{b}) = \zeta(u)\zeta(v) = \zeta(u*v)\,.$$

It remains only to show that every word appearing in $u*v$ is of weight $n+m = wt(u)+wt(v)$. We prove this by induction on $r+s$, as usual. If one of u or v is 1 then w.l.o.g. $u=1 \implies u*v=v$

of weight m. Since $\mathbf{a} = \varnothing$ we have $n + m = m$ as required.

Now assume the claim holds for all $r + s \leq k$ fixed, and take $u = z_{a_1} \dots z_{a_r} = z_{a_1} u', v = z_{b_1} \dots z_{b_s} = z_{b_1} v'$ with $r + s = k + 1$. We have

$$u * v = z_{a_1}(u' * v) + z_{b_1}(u * v') + z_{a_1+b_1}(u' * v')$$

and by the induction step, all words u_i appearing in $u' * v$ satisfies

$$wt(u_i) = wt(u') + wt(v) = a_2 + \dots + a_r + m\,.$$

Appending to u_i the letter z_{a_1} as in $z_{a_1}(u' * v)$, we obtain

$$wt(z_{a_1} u_i) = a_1 + a_2 + \dots + a_r + m = n + m$$

as required. The other two terms are almost identical, so the induction step is complete. Finally $u * v$ is a sum of words w_i of weight $n + m$, so that $\zeta(\mathbf{a})\zeta(\mathbf{b}) = \zeta(u * v)$ is a sum (by linear extension) of MZVs of weight $n + m$. Since $\mathcal{Z}_{n+m}$ is a vector space, we obtain $\zeta(\mathbf{a})\zeta(\mathbf{b}) \in \mathcal{Z}_{n+m}$ which completes the proof. □

Proposition 2.3.4. ($\star$) For any admissible multi-indices $\mathbf{a}, \mathbf{b}$ of weights n, m respectively,

$$\zeta(\mathbf{a})\zeta(\mathbf{b}) = \sum_{\sigma \in \mathrm{Sh}(n,m)} \zeta\left(\sigma^{-1}\left(\bar{\mathbf{a}}\bar{\mathbf{b}}\right)\right)\,.$$

Proof. The product is

$$\zeta(\mathbf{a})\zeta(\mathbf{b}) = \int\limits_{\Delta^n} \omega_{\alpha_1}(t_1) \cdots \omega_{\alpha_n}(t_n) \int\limits_{\Delta^m} \omega_{\beta_1}(t_1) \cdots \omega_{\beta_m}(t_m)$$

$$= \int\limits_{\Delta^n \times \Delta^m} \omega_{\alpha_1}(t_1) \cdots \omega_{\alpha_n}(t_n)\, \omega_{\beta_1}(t_{n+1}) \cdots \omega_{\beta_m}(t_{n+m})$$

where $\Delta^n = \{(t_1, \dots, t_n) \in \mathbb{R}^n \mid 1 > t_1 > \dots > t_n > 0\}$. We now sum over all possible orderings of t_i and t_j coming from Δ^n and Δ^m, while respecting initial orders. Each ordering where all choices are strict (i.e. there are no $t_i = t_j$) can be written as

$$t_{i_1} > \dots > t_{i_{n+m}}$$

with $i_j \in (1, \dots n + m)$ all distinct. This corresponds precisely to a permutation of $t_1 > \dots > t_{n+m}$, so we can write $i_j = \tau(j)$ for some $\tau \in S_{n+m}$. Note that the new location of t_j in the ordering is at position $\tau^{-1}(j)$: considering the example $\tau = (123)$, the new permutation is

$$t_2 > t_3 > t_1$$

and the location of t_1 is at position $\tau^{-1}(1) = 3$, *not* $\tau(1)$!

Respecting initial orders means that we must still have $t_1 > \ldots > t_n$ and $t_{n+1} > \ldots > t_{n+m}$ in the permutation. Following the note above, this happens exactly when $\tau^{-1}(1) < \ldots < \tau^{-1}(n)$ and $\tau^{-1}(n+1) < \ldots < \tau^{-1}(n+m)$, i.e. when $\tau^{-1} \in \mathrm{Sh}(n,m)$. Writing $\sigma = \tau^{-1}$, this gives us the following decomposition into orderings:

$$\begin{aligned}\Delta^n \times \Delta^m &= \bigcup_{\sigma \in \mathrm{Sh}(n,m)} \{(t_1, \ldots, t_{n+m}) \in \mathbb{R}^{n+m} \mid 1 > t_{\sigma^{-1}(1)} > \ldots > t_{\sigma^{-1}(n+m)} > 0\} \cup \bigcup_i U_i \\ &\coloneqq \bigcup_{\sigma \in \mathrm{Sh}(n,m)} \Delta_\sigma \cup \bigcup_i U_i\end{aligned}$$

for some finite number of domains U_i of dimension strictly less than $n+m$, as they come from equating certain t_i. Now the integral of a function in n variables over a k-dimensional domain is 0 if $k \leq n-1$ [This is a simple generalisation of the 1-dimensional case, where integrating over a point is zero: $\int_a^a f(x)dx = 0$]. Note that these extra pieces U_i were also present in the stuffle product as the third terms '$n_i = m_j$', but could not be ignored. For the product of integrals, these can be dismissed since they contribute 0 to the integral.

Writing $\bar{\mathbf{a}}\bar{\mathbf{b}} = \alpha_1 \ldots \alpha_n \beta_1 \ldots \beta_m \coloneqq \epsilon_1 \ldots \epsilon_{n+m}$ and reordering the ω, we obtain for each σ:

$$\begin{aligned}\int_{\Delta_\sigma} & \omega_{\alpha_1}(t_1) \cdots \omega_{\alpha_n}(t_n)\, \omega_{\beta_1}(t_{n+1}) \cdots \omega_{\beta_m}(t_{n+m}) \\ &= \int\limits_{1 > t_{\sigma^{-1}(1)} > \ldots > t_{\sigma^{-1}(n+m)} > 0} \omega_{\epsilon_1}(t_1) \cdots \omega_{\epsilon_{n+m}(t_{n+m})} \\ &= \int\limits_{1 > t_{\sigma^{-1}(1)} > \ldots > t_{\sigma^{-1}(n+m)} > 0} \omega_{\epsilon_{\sigma^{-1}(1)}}(t_{\sigma^{-1}(1)}) \cdots \omega_{\epsilon_{\sigma^{-1}(n+m)}}(t_{\sigma^{-1}(n+m)}) \\ &= \zeta(\epsilon_{\sigma^{-1}(1)} \ldots \epsilon_{\sigma^{-1}(n+m)}) \\ &= \zeta(\sigma^{-1}(\epsilon_1 \ldots \epsilon_{n+m})) \\ &= \zeta(\sigma^{-1}(\bar{\mathbf{a}}\bar{\mathbf{b}}))\,.\end{aligned}$$

Finally, using our decomposition of $\Delta^n \times \Delta^m$ we conclude:

$$\begin{aligned}\zeta(\mathbf{a})\zeta(\mathbf{b}) &= \int\limits_{\Delta^n \times \Delta^m} \omega_{\alpha_1}(t_1) \cdots \omega_{\alpha_n}(t_n)\, \omega_{\beta_1}(t_{n+1}) \cdots \omega_{\beta_m}(t_{n+m}) \\ &= \sum_{\sigma \in \mathrm{Sh}(n,m)} \int_{\Delta_\sigma} \omega_{\alpha_1}(t_1) \cdots \omega_{\alpha_n}(t_n)\, \omega_{\beta_1}(t_{n+1}) \cdots \omega_{\beta_m}(t_{n+m}) \\ &= \sum_{\sigma \in \mathrm{Sh}(n,m)} \zeta(\sigma^{-1}(\bar{\mathbf{a}}\bar{\mathbf{b}}))\,. \qquad \square\end{aligned}$$

A.3 Chapter 3

Theorem 3.1.3 (Duality). ($\star$) For any word $w \in \mathfrak{h}^0$,

$$\zeta(\tau(w)) = \zeta(w)\,.$$

Proof. Writing $w = \epsilon_1 \dots \epsilon_n$ with $\epsilon_i \in \{x, y\}$, we have $\tau(w) = \tau(\epsilon_n) \dots \tau(\epsilon_1)$. Then

$$\zeta(w) = \int\limits_{1>t_1>\dots>t_n>0} \omega_{\epsilon_1}(t_1) \cdots \omega_{\epsilon_n}(t_n)$$

and

$$\zeta(\tau(w)) = \int\limits_{1>t_1>\dots>t_n>0} \omega_{\tau(\epsilon_n)}(t_1) \cdots \omega_{\tau(\epsilon_1)}(t_n)$$

by Kontsevich. We apply the change of variables $s_i = 1 - t_{n+1-i}$ to the first integral, with $dt_i = -ds_{n+1-i}$. The domain $\{1 > t_1 > \dots > t_n > 0\}$ is sent to $\{1 > 1 - s_n > \dots > 1 - s_1 > 0\} = \{1 > s_1 > \dots > s_n > 0\}$, but we must be careful with the resulting orientation of this new domain. Defining t_{n+1} and parametrising the original domain with t_i running from t_{i+1} to 1, the interated integral is

$$\begin{aligned}\zeta(w) &= \int\limits_{1>t_1>\dots>t_n>0} \omega_{\epsilon_1}(t_1) \cdots \omega_{\epsilon_n}(t_n) \\ &= \int_0^1 \int_{t_n}^1 \cdots \int_{t_2}^1 \omega_{\epsilon_1}(t_1) \cdots \omega_{\epsilon_n}(t_n)\,.\end{aligned}$$

Schematically, we have

$$t_i : \quad t_{i+1} \quad \mapsto \quad 1\,.$$

The change of variables gives

$$s_i = 1 - t_{n+1-i} : \quad 1 - t_{n+1-i+1} = s_{i-1} \quad \mapsto \quad 1 - 1 = 0\,,$$

which is 'reversed' in the sense that s_i *decreases* from s_{i-1} to 0, which is in the opposite direction of t_i *increasing* from t_{i+1} to 1. More precisely, remembering that $dt_i = -ds_{n+1-i}$, we obtain

$$\begin{aligned}\zeta(w) &= (-1)^n \int_1^0 \int_{s_2}^0 \cdots \int_{s_{n-1}}^0 \omega_{\epsilon_1}(1 - s_n) \cdots \omega_{\epsilon_n}(1 - s_1) \\ &= \int_0^1 \int_0^{s_2} \cdots \int_0^{s_{n-1}} \omega_{\epsilon_1}(1 - s_n) \cdots \omega_{\epsilon_n}(1 - s_1)\end{aligned}$$

where we have flipped the integrals in such a way that all s_i now increase. The iterated integral converges (to an MZV) by Kontsevich's theorem, and all the integrands are positive in the region of integration, so the integral converges absolutely. By Fubini's Theorem, we can swap the order of integration. The domain is the standard open n-simplex $\Delta^n = \{1 > s_1 > \dots > s_n > 0\}$ which we have re-oriented positively, so we can parametrise it as we did with the t_i. Swapping the ω accordingly gives

$$\begin{aligned}\zeta(w) &= \int_0^1 \int_{s_n}^1 \cdots \int_{s_2}^1 \omega_{\epsilon_n}(1-s_1)\cdots\omega_{\epsilon_1}(1-s_n) \\ &= \int\limits_{1>s_1>\ldots>s_n>0} \omega_{\epsilon_n}(1-s_1)\cdots\omega_{\epsilon_1}(1-s_n)\,.\end{aligned}$$

It remains only to note that

$$\begin{aligned}\omega_x(t) &= \frac{1}{t} &&\implies && \omega_x(1-t) = \omega_y(t) \\ \omega_y(t) &= \frac{1}{1-t} &&\implies && \omega_y(1-t) = \omega_x(t)\,,\end{aligned}$$

which implies

$$\omega_{\epsilon_i}(1-t) = \omega_{\tau(\epsilon_i)}(t)$$

for all $\epsilon_i \in \{x,y\}$. Applying this equality gives the result

$$\zeta(w) = \int\limits_{1>s_1>\ldots>s_n>0} \omega_{\tau(\epsilon_n)}(s_n)\cdots\omega_{\tau(\epsilon_1)}(s_1) \;=\; \zeta(\tau(w))\,. \qquad \square$$

Corollary 3.1.6. ($\star$) For all $k \geq 3$, we have

$$\dim(\mathcal{Z}_k) \leq \begin{cases} 2^{k-3} & \text{if } k \text{ is odd} \\ 2^{k-3} + \frac{1}{2}\binom{k-2}{k/2-1} & \text{if } k \text{ is even.}\end{cases}$$

Proof. To begin, the more elegant proof of Proposition 1.4.6 goes as follows. By our binary sequence correspondence (harmonic algebra), the number of admissible multi-indices of weight $k \geq 2$ is the number of binary sequences

$$x\epsilon_2 \ldots \epsilon_{k-1} y$$

with $\epsilon_i \in \{x,y\}$ for all i, which is 2^{k-2}. This makes counting elements of a particular length much easier as well, since length is the number of y's in the above sequence. We already have on y guaranteed at the end, so the number of elements of fixed length $1 \leq a \leq k-1$ is

$$\binom{k-2}{a-1}.$$

Write $\delta(k) = 0$ if k odd, 1 otherwise. Then the number of elements of length strictly smaller than $k/2$ is

$$\begin{aligned}\sum_{a=1}^{k/2-1}\binom{k-2}{a-1} &= \sum_{a=0}^{k/2-2}\binom{k-2}{a}\\ &= \sum_{a=0}^{k-2}\binom{k-2}{a} - \delta(k)\binom{k-2}{k/2-1} - \sum_{a=k/2}^{k-2}\binom{k-2}{a}\\ &= (1+1)^{k-2} - \delta(k)\binom{k-2}{k/2-1} - \sum_{a=k/2}^{k-2}\binom{k-2}{k-2-a}\\ &= 2^{k-2} - \delta(k)\binom{k-2}{k/2-1} - \sum_{b=0}^{k/2-2}\binom{k-2}{b}\end{aligned}$$

with change of variables $b = k-2-a$. Comparing the first and last lines, we obtain

$$\sum_{a=1}^{k/2-1}\binom{k-2}{a-1} = 2^{k-3} - \frac{\delta(k)}{2}\binom{k-2}{k/2-1}.$$

Taking any MZV $\zeta(\mathbf{a})$ of length r strictly smaller than $k/2$, we have by Proposition 3.1.2 that $\zeta(\mathbf{a}) = \zeta(\tau(\mathbf{a}))$ with dual length being $k-r > k/2$. Hence every MZV of length below half is equal to one of length above half, which folds the dimension in half *except* for MZVs of length $k/2$ exactly, for k even. More precisely, removing all MZVs of length strictly smaller than $k/2$ gives

$$\dim_(\mathcal{Z}_k) \le 2^{k-2} - \left[2^{k-3} - \frac{\delta(k)}{2}\binom{k-2}{k/2-1}\right] = 2^{k-3} + \frac{\delta(k)}{2}\binom{k-2}{k/2-1}$$

as claimed. □

Remark. We can also prove the odd case by splitting in terms of even/odd length rather than greater/smaller than half. This yields greater insight into how we view the folded space, so we make this rigorous as follows. Using the binomial theorem, the number of even-length elements is

$$\begin{aligned}\sum_{a=1 \text{ even}}^{k-1}\binom{k-2}{a-1} = \sum_{a=0 \text{ even}}^{k-2}\binom{k-2}{a} &= \sum_{a=0}^{k-2}\binom{k-2}{a}\frac{1+(-1)^a}{2}\\ &= \frac{1}{2}\sum_{a=0}^{k-2}\binom{k-2}{a} + \frac{1}{2}\sum_{a=0}^{k-2}\binom{k-2}{a}(-1)^a\\ &= \frac{1}{2}(1+1)^{k-2} + \frac{1}{2}(1-1)^{k-2} = 2^{k-3},\end{aligned}$$

where $0^{k-2} = 0$ because $k \ge 3$ by assumption. Thus, we have an equal number of even- and odd-length MZVs. For k odd, take any MZV $\zeta(\mathbf{a})$ of odd length r. Then Proposition 3.1.2 states that $\zeta(\mathbf{a}) = \zeta(\tau(\mathbf{a}))$ with the dual length being $k-r$, which is even. Hence every odd-length MZV is equal to an even-length one, and therefore folds the space in half:

$$\dim(\mathcal{Z}_k) \le 2^{k-2} - 2^{k-3} = 2^{k-3}.$$

Proposition 3.3.8. ($\star$) For any words $u, w \in \mathfrak{h}^1$ with $l(w) = r$,

$$u \cdot w = L_r(u * w)\,.$$

Proof. By induction on r. If $u = 1$, we trivially have

$$u \cdot w = w = L_0(w) = L_0(u * w)\,,$$

so we can take $u \neq 1$ and write $u = z_{b_1} \dots z_{b_s}$ with $l(u) = s > 0$. For $r = 0$,

$$u \cdot w = 0 = L_0(u) = L_0(u * w)\,.$$

For $r = 1$, write $w = z_a$. If $s = 1$ then

$$u \cdot w = z_{a+b_1} = L_1(z_{b_1} z_a + z_a z_{b_1} + z_{a+b_1}) = L_1(u * w)\,.$$

Otherwise, we have $l(u) > 1$ and a routine induction gives

$$u \cdot w = 0 = L_1(z_{b_1}(z_a * u) + z_a u + z_{a+b_1} z_{b_2} \dots z_{b_s}) = L_1(u * w)\,.$$

For the induction step, write $w = z_{a_1} w'$ with $r \geq 2$, $u = z_{b_1} u'$, possibly with $u' = 1$. Then

$$\begin{aligned} L_r(u * w) &= L_r(z_{b_1}(u' * w) + z_{a_1}(u * w') + z_{a_1+b_1}(u' * w')) \\ &= z_{b_1} L_{r-1}(u' * w) + z_{a_1} L_{r-1}(u * w') + z_{a_1+b_1} L_{r-1}(u' * w') \\ &= z_{a_1} L_{r-1}(u * w') + z_{a_1+b_1} L_{r-1}(u' * w') \end{aligned}$$

with the first term vanishing since all words in $u' * w$ have length at least r, given that w has length r (routine induction). On the other hand, note that

$$\Delta(u) = \sum_{j=0}^{s} z_{b_1} \dots z_{b_j} \otimes z_{b_{j+1}} \dots z_{b_s}\,.$$

Using the induction step, this gives us

$$\begin{aligned} u \cdot w &= \sum_{u_1 \otimes u_2 \in \Delta(u)} (u_1 \cdot z_{a_1})(u_2 \cdot w') \\ &= \sum_{u_1 \otimes u_2 \in \Delta(u)} L_1(u_1 * z_{a_1}) L_{r-1}(u_2 * w') \\ &= L_1(1 * z_{a_1}) L_{r-1}(u * w') + L_1(z_{b_1} * z_{a_1}) L_{r-1}(u' * w') \\ &= z_{a_1} L_{r-1}(u * w') + z_{a_1+b_1} L_{r-1}(u' * w') \\ &= L_r(u * w) \end{aligned}$$

since all other terms u_1 in $\Delta(u)$ have length strictly greater than 1. $\square$

Proposition 3.3.10. ($\star$) For all words $w = z_{a_1} \dots z_{a_r} \in \mathfrak{h}^1$ and $n \geq 0$ we have

$$h_n \cdot w = \sum_{\substack{c_1 + \dots + c_r = n \\ c_i \geq 0}} z_{a_1+c_1} \dots z_{a_r+c_r}\,.$$

Proof. By induction on length r. For $n = 0$ the claim is trivial, so take $n \geq 1$. For $r = 0$ we define the RHS to be 0, and the LHS agrees by the fourth remark. For $r = 1$ we have by proposition 3.3.8 that

$$\begin{aligned} h_n \cdot z_{a_1} &= \sum_{v \in W_n} (v \cdot z_{a_1}) = \sum_{v \in W_n} L_1(v * z_{a_1}) \\ &= z_n \cdot z_{a_1} = z_{a_1+n} \end{aligned}$$

since all words in W_n have length greater than 1 except z_n. For the induction step, write $w = z_{a_1} w'$ and for each $v \in W_n$, write $v = z_{b_1} v'$ (possibly with $v' = 1$). Then

$$\begin{aligned} h_n \cdot w &= \sum_{v \in W_n} L_r(v * w) \\ &= \sum_{v \in W_n} z_{b_1} L_{r-1}(v' * w) + z_{a_1} L_{r-1}(v * w') + z_{a_1+b_1} L_{r-1}(v' * w') \\ &= \sum_{v \in W_n} z_{a_1}(v \cdot w') + z_{a_1+b_1}(v' \cdot w') \\ &= z_{a_1}(h_n \cdot w') + \sum_{v \in W_n} z_{a_1+b_1}(v' \cdot w') \, . \end{aligned}$$

We now split $W_n = \{z_{b_1} \dots z_{b_s} \in \mathfrak{h}^1 \mid b_1 + \dots + b_s = n\}$ into

$$W_n = \bigsqcup_{c_1=1}^{n} W_{n,c_1} := \bigsqcup_{c_1=1}^{n} \{z_{b_1} \dots z_{b_s} \in \mathfrak{h}^1 \mid b_1 + \dots + b_s = n, b_1 = c_1\} \, ,$$

and we notice that $W_{n,c_1} = \{z_{b_1} u \mid u \in W_{n-c_1}\}$. This gives us

$$\begin{aligned} h_n \cdot z_{a_1} &= z_{a_1}(h_n \cdot w') + \sum_{c_1=1}^{n} \sum_{v \in W_{n,c_1}} z_{a_1+b_1}(v' \cdot w') \\ &= z_{a_1}(h_n \cdot w') + \sum_{c_1=1}^{n} \sum_{u \in W_{n-c_1}} z_{a_1+c_1}(u \cdot w') \\ &= \sum_{c_1=0}^{n} \sum_{u \in W_{n-c_1}} z_{a_1+c_1}(u \cdot w') \\ &= \sum_{c_1=0}^{n} z_{a_1+c_1}(h_{n-c_1} \cdot w') \\ &= \sum_{c_1=0}^{n} z_{a_1+c_1} \sum_{\substack{c_2+\dots+c_r=n-c_1 \\ c_i \geq 0}} z_{a_2+c_2} \dots z_{a_r+c_r} \\ &= \sum_{\substack{c_1+c_2+\dots+c_r=n \\ c_i \geq 0}} z_{a_1+c_1} \dots z_{a_r+c_r} \end{aligned}$$

and the proof is complete. □

A.4 Chapter 4

Proposition 4.2.6. ($\star$) Let $Z^t = Z \circ S^t : \mathfrak{h}^0[t] \longrightarrow \mathbb{R}[t]$. Then

$$Z^t(z_{a_1} \dots z_{a_r}) = \zeta^t(a_1, \dots, a_r)\,.$$

Proof. We prove that

$$S^t(z_{a_1} \dots z_{a_r}) = \sum_{w \in W} t^{\sigma(w)} w$$

where $W = \{(z_{a_1} \square \dots \square\, z_{a_r}) \mid \square \in \{\circ, \cdot\}\}$ analogous to P and $\sigma(w)$ the number of $\circ$ used in w, analogous to $\sigma(\mathbf{p})$. Note that $\circ$ corresponds to addition in multi-indices, whereas concatenation $\cdot$ corresponds to inserting a comma.

We prove this claim by induction on length r. For the base case $r = 1$ we have $W = \{z_{a_1}\}$ and $\sigma(z_{a_1}) = 0$, so the RHS is $0^0 z_{a_1} = z_{a_1}$. The LHS is

$$S^t(z_{a_1}) = z_{a_1} S^t(1) + t z_{a_1} \circ S^t(1) = z_{a_1}$$

in agreement. For the induction step, let $W' = \{(z_{a_2} \square \dots \square\, z_{a_r}) \mid \square \in \{\circ, \cdot\}\}$ and decompose

$$W = W_1 \sqcup W_2 := \{z_{a_1} w \mid w \in W'\} \sqcup \{z_{a_1} \circ w \mid w \in W'\}\,.$$

Then $\sigma(z_{a_1} w) = \sigma(w)$ and $\sigma(z_{a_1} \circ w) = \sigma(w) + 1$ for $w \in W'$, from which we obtain:

$$\begin{aligned} S^t(z_{a_1} \dots z_{a_r}) &= z_{a_1} S^t(z_{a_2} \dots z_{a_r}) + t z_{a_1} \circ S^t(z_{a_2} \dots z_{a_r}) \\ &= \sum_{w \in W'} t^{\sigma(w)} z_{a_1} w + \sum_{w \in W'} t^{\sigma(w)+1} z_{a_1} \circ w \\ &= \sum_{w \in W_1} t^{\sigma(w)} w + \sum_{w \in W_2} t^{\sigma(w)} w \\ &= \sum_{w \in W} t^{\sigma(w)} w \end{aligned}$$

which concludes the induction. Finally,

$$\begin{aligned} Z^t(z_{a_1} \dots z_{a_r}) = Z \circ S^t(z_{a_1} \dots z_{a_r}) = \sum_{w \in W} t^{\sigma(w)} Z(w) = \sum_{\mathbf{p} \in P} t^{\sigma(\mathbf{p})} \zeta(\mathbf{p}) \\ = \zeta^t(a_1, \dots, a_r)\,. \end{aligned}$$

□

Proposition 4.2.8. ($\star$) For any odd $n \geq 1$,

$$\zeta^{-1}(2, \{1\}^n) = 0\,.$$

Proof. Let $u = z_2 \underbrace{z_1 \dots z_1}_{n} = z_2 z_1^n \in \mathfrak{h}^0$ the corresponding word. We have shown in the proof of Proposition 4.2.6 that

$$S^t(u) = \sum_{w \in W} t^{\sigma(w)} w$$

where $W = \{(z_2\Box\underbrace{z_1\Box\ldots\Box z_1}_{n}) \mid \Box \in \{\circ, \cdot\}\}$ and $\sigma(w) = l(u) - l(w)$. Now

$$z_m \circ u = x^m u$$

for any integer $m \geq 1$ and word $u \in \mathfrak{h}^1$, so we can rewrite $W = \{(xa_1 \ldots a_n y \mid a_i \in \{x, y\}\}$ and $\sigma(w) = n + 1 - l(w)$. Notice that for any word $w = xa_1 \ldots a_n y \in W$, we have

$$\tau(w) = x\tau(a_n) \ldots \tau(a_1)y \in W\,.$$

For n odd, Proposition 3.1.2 implies that

$$\sigma(\tau(w)) = n + 1 - l(\tau(w)) = n + 1 - (n + 2 - l(w)) = n - (n + 1 - l(w)) = n - \sigma(w)\,,$$

which cannot have the same parity as $\sigma(w)$, since otherwise n is even. It follows that $\tau(w) \neq w$, which splits the set W in disjoint and bijective sets W_1, W_2 such that $w \in W_1 \iff \tau(w) \in W_2$. Now taking $t = -1$ implies that

$$t^{\sigma(w)} = (-1)^{\sigma(w)} = -(-1)^{\sigma(\tau(w))}$$

$\sigma(w)$ and $\sigma(\tau(w))$ are not of the same parity. By the duality theorem, we finally obtain that

$$\begin{aligned}
\zeta^{-1}(2, \{1\}^n) &= \zeta^{-1}(u) \\
&= \sum_{w\in W_1} (-1)^{\sigma(w)}\zeta(w) + \sum_{w\in W_2} (-1)^{\sigma(w)}\zeta(w) \\
&= \sum_{w\in W_1} (-1)^{\sigma(w)}\zeta(w) + (-1)^{\sigma(\tau(w))}\zeta(\tau(w)) \\
&= \sum_{w\in W_1} (-1)^{\sigma(w)}\zeta(w) - (-1)^{\sigma(w)}\zeta(w) \\
&= 0\,.
\end{aligned}$$

□

Lemma 4.3.6. ($\star$) For any letters $a, b \in \mathcal{A}$ and words $u, v \in \mathfrak{h}^1$, the following equalities hold.

$$(a \circ u) * (bv) = a \circ (u * bv) + b((a \circ u) * v) - (a \circ b)(u * v) \tag{1}$$
$$(au) * (b \circ v) = b \circ (au * v) + a(u * (b \circ v)) - (a \circ b)(u * v) \tag{2}$$
$$(a \circ u) * (b \circ v) = a \circ (u * (b \circ v)) + b \circ ((a \circ u) * v) - (a \circ b) \circ (u * v) \tag{3}$$
$$S^t(a \circ u) = a \circ S^t(u)\,.. \tag{4}$$

Proof. We first prove (4). For $a \in \mathcal{A}$ and $u = bu' \in \mathfrak{h}^1$ with $b \in \mathcal{A}$ we have

$$\begin{aligned}
S^t(a \circ u) &= S^t((a \circ b)u') = (a \circ b)S^t(u') + t(a \circ b) \circ S^t(u') \\
&= a \circ (bS^t(y') + tb \circ S^t(u')) = a \circ S^t(u)\,.
\end{aligned}$$

This also holds for $w = 1$, so the proof is complete. We now turn to the other three, proceeding by induction on $l(u) + l(v)$. If w.l.o.g. $u = 1$, we have $a \circ u = 0$ implying

$$(a \circ u) * (bv) = a \circ bv - (a \circ b)v \qquad (1)$$
$$(a \circ u) * (b \circ v) = 0 = a \circ (b \circ v) - (a \circ b) \circ v\,. \qquad (3)$$

For equation (2), we can perform induction on $l(v)$ to obtain the result. For $v = 1$ the claim is trivial. For $l(v) \geq 1$, the proof is just a simpler case of taking u and v both not 1, i.e. $l(u) + l(v) \geq 2$. We thus proceed to the induction step on $l(u) + l(v) \geq 2$, writing $u = cu'$ and $v = dv'$. Then

$$\begin{aligned}(a \circ u) * (bv) &= (a \circ c)(u' * bv) + b((a \circ u) * v) + (a \circ c \circ b)(u' * v)\\ a \circ (u * bv) &= (a \circ c)(u' * bv) + (a \circ b)(u * v) + (a \circ c \circ b)(u' * v)\,,\end{aligned}$$

and comparing the two gives equation (1). For equation (2), swapping a with b and u with v gives the result by using commutativity of the shuffle product. Finally,

$$\begin{aligned}(a \circ u) * (b \circ v) &= (a \circ c)(u' * (b \circ v)) + (b \circ d)((a \circ u) * v') + (a \circ c \circ b \circ d)(u' * v')\\ a \circ (u * (b \circ v)) &= (a \circ c)(u' * (b \circ v)) + (a \circ b \circ d)(u * v') + (a \circ c \circ b \circ d)(u' * v')\\ b \circ ((a \circ u) * v) &= (b \circ a \circ c)(u' * v) + (b \circ d)((a \circ u) * v') + (a \circ c \circ b \circ d)(u' * v')\\ (a \circ b) \circ (u * v) &= (a \circ b \circ c)(u' * v) + (a \circ b \circ d)(u * v') + (a \circ c \circ b \circ d)(u' * v')\,.\end{aligned}$$

Adding the second and third line and subtracting the fourth gives the first, using commutativity of the circle product. This is equation (3) and concludes the proof. □

Theorem 4.3.5. ($\star$) The map $S^t : (\mathfrak{h}^1[t], \overset{t}{*}) \longrightarrow (\mathfrak{h}^1[t], *)$ is a homomorphism.

Proof. We need to show that

$$S^t(w \overset{t}{*} w') = S^t(w) * S^t(w')$$

for all words $w, w' \in \mathfrak{h}^1[t]$, which we prove by induction on the sum of lengths $r + s$. If one of w, w' is 1 then the claim is trivial since $w \overset{t}{*} 1 = w = w * 1$. Otherwise, write $w = au, w' = bv$ with $a, b \in \mathcal{A}$. We abuse notation by defining $(a + b\circ)u = au + b \circ u$, so that $S^t(au) = (a + ta\circ)u$. Then

$$\begin{aligned}S^t(w \overset{t}{*} w') &= S^t(a(u \overset{t}{*} bv)) + S^t(b(au \overset{t}{*} v)) + (1 - 2t)S^t((a \circ b)(u \overset{t}{*} v)) + (t^2 - t)S^t((a \circ b) \circ (u \overset{t}{*} v))\\ &= (a + ta\circ)(S^t(u) * S^t(bv))\\ &\quad + (b + tb\circ)(S^t(au) * S^t(v))\\ &\quad + (1 - 2t)(a \circ b + t(a \circ b)\circ)(S^t(u) * S^t(v))\\ &\quad + (t^2 - t)S^t((a \circ b) \circ (u \overset{t}{*} v))\end{aligned}$$

using the induction step. Then writing $S^t(u) = U$ and $S^t(v) = V$, we use equation (4) to obtain

$$\begin{aligned}S^t(w \overset{t}{*} w') &= (a + ta\circ)(U * bV + tU * (b \circ V))\\ &\quad +(b + tb\circ)(aU * V + t(a \circ U) * V)\\ &\quad +(1 - 2t)(a \circ b + t(a \circ b)\circ)(U * V)\\ &\quad +(t^2 - t)(a \circ b) \circ (U * V)\\ &= (a + ta\circ)(U * bV + tU * (b \circ V))\\ &\quad +(b + tb\circ)(aU * V + t(a \circ U) * V)\\ &\quad +(1 - 2t)(a \circ b)(U * V) - t^2(a \circ b) \circ (U * V)\,.\end{aligned}$$

On the other hand,

$$\begin{aligned}S^t(w) * S^t(w') &= ((a + ta\circ)U) * ((b + tb\circ)V)\\ &= a(U * bV) + b(aU * V) + (a \circ b)(U * V)\\ &\quad + t(a \circ U) * (bV) + t(aU) * (b \circ V)\\ &\quad + t^2(a \circ U) * (b \circ V)\,.\end{aligned}$$

We now use Lemma 4.3.6 on all terms of the second and third lines to obtain

$$\begin{aligned}S^t(w) * S^t(w') &= a(U * bV) + b(aU * V) + (a \circ b)(U * V)\\ &\quad + t\,[a \circ (U * bV) + b((a \circ U) * V) - (a \circ b)(U * V)]\\ &\quad + t\,[b \circ (aU * V) + a(U * (b \circ V)) - (a \circ b)(U * V)]\\ &\quad + t^2\,[a \circ (U * (b \circ V)) + b \circ ((a \circ U) * V) - (a \circ b) \circ (U * V)]\\ &= (a + ta\circ)(U * bV + tU * (b \circ V))\\ &\quad +(b + tb\circ)(aU * V + t(a \circ U) * V)\\ &\quad +(a \circ b)(U * V) - 2t(a \circ b)(U * V) - t^2(a \circ b) \circ (U * V)\\ &= S^t(w \overset{t}{*} w')\,,\end{aligned}$$

which concludes our proof! ☐

Proposition 4.3.9. ($\star$) The t-stuffle is associative, commutative and respects weight.

Proof. By Proposition 2.2.11, the stuffle product is associative and commutative, which implies that

$$\begin{aligned}S^t((u \overset{t}{*} v)) \overset{t}{*} w) &= S^t(u \overset{t}{*} v) * S^t(w) = (S^t(u) * S^t(v)) * S^t(w)\\ &= S^t(u) * (S^t(v) * S^t(w)) = S^t(u) * S^t(v \overset{t}{*} w) = S^t(u \overset{t}{*} (v \overset{t}{*} w))\,.\end{aligned}$$

Now taking the inverse S^{-t} on both sides gives us associativity

$$(u \overset{t}{*} v) \overset{t}{*} w = u \overset{t}{*} (v \overset{t}{*} w)\,,$$

and commutativity is proved almost identically.

Moreover, the stuffle respects weight by Corollary 2.2.19, and so does S^t for all t. Therefore all words appearing in $u * v$ have weight $wt(u) + wt(v)$, and so all words appearing in $S^t(u \overset{t}{*} v) = S^t(u) * S^t(v)$ have weight $wt(S^t(u)) + wt(S^t(v)) = wt(u) + wt(v)$. Using the inverse S^{-t}, all words appearing in $u \overset{t}{*} v$ must have weight $wt(u) + wt(v)$ and we conclude that the t-stuffle also respects weight. ☐

Proposition 4.4.8. ($\star$) For any word $w = uy \in \mathfrak{h}^1[t]$, the map S^t satisfies

$$S^t(uy) = R^t(u)y\,.$$

Proof. By induction on length. The case $w = 1$ does not apply, so the base case is $w = z_{a_1} = x^{a_1-1}y$, for which

$$S^t(w) = z_{a_1} = x^{a_1-1}y = R^t(x^{a_1-1})y\,.$$

For the induction step, take any word $w = z_{a_1} \dots z_{a_r} = z_{a_1}v = uy$ with $r \geq 2$, and write $v = v'y$. Then

$$\begin{aligned} S^t(w) &= z_{a_1}S^t(v) + tz_{a_1} \circ S^t(v) \\ &= z_{a_1}R^t(v')y + tz_{a_1} \circ R^t(v')y \\ &= x^{a_1-1}yR^t(v')y + tx^{a_1-1}xR^t(v')y \\ &= x^{a_1-1}(y + tx)R^t(v')y \\ &= R^t(z_{a_1})R^t(v')y \\ &= R^t(u)y\,. \end{aligned}$$

□

Theorem 4.4.6. (⋆) The map $S^t : (\mathfrak{h}^1[t], \overset{t}{ш}) \longrightarrow (\mathfrak{h}^1[t], ш)$ is a homomorphism.

Proof. We need to show that

$$S^t(w \overset{t}{ш} w') = S^t(w) \, ш \, S^t(w')$$

for all words $w, w' \in \mathfrak{h}^1[t]$. Proceed by induction on the sum of weights n, m. If one of w, w' is 1, the claim is trivial since $w \overset{t}{ш} 1 = w = w \, ш \, 1$, so we can take $n, m \geq 1$. As foreshadowed by the t-shuffle formula, the case where at least one of n, m is 1 behaves differently due to the delta terms. For $n = m = 1$ we have $w = w' = y$, so that

$$\begin{aligned} S^t(y \overset{t}{ш} y) &= S^t(2yy - 2txy) \\ &= 2[yS^t(y) + ty \circ S^t(y) - txy] \\ &= 2yy = y \, ш \, y = S^t(y) \, ш \, S^t(y) \end{aligned}$$

as required. For $n > 1$ and $m = 1$, write $w = au$ with $u \neq 1$ and $w' = 1$. By induction on n,

$$\begin{aligned} S^t(au \overset{t}{ш} y) &= S^t(a(u \overset{t}{ш} y) + yau - txau) \\ &= R^t(a)S^t(u \overset{t}{ш} y) + R^t(y)S^t(au) - tR^t(x)S^t(au) \\ &= R^t(a)(S^t(u) \, ш \, S^t(y)) + yS^t(au) \\ &= R^t(a)(S^t(u) \, ш \, S^t(y)) + S^t(y)(R^t(a)S^t(u) \, ш \, 1) \\ &= (R^t(a)S^t(u) \, ш \, S^t(y)) \\ &= S^t(au) \, ш \, S^t(y)\,. \end{aligned}$$

One may ask why the penultimate equality holds, considering that the shuffle product is recursive on letters, and $R^t(a)$ may not be a letter. This is true, but a being a letter implies that $a = x$ or $a = y$, giving $R^t(a) = x$ (a letter) or $R^t(a) = y + tx$. The latter splits into letters by $\mathbb{Q}[t]$-linearity of the shuffle product, so the result holds as well.

By commutativity the case $n = 1$ and $m > 1$ is identical, so we proceed to the case $n, m > 1$. Write $w = au, w' = bv$ with $u, v \neq 1$. Then

$$\begin{aligned} S^t(w \overset{t}{\sqcup\!\sqcup} w') &= S^t(a(u \overset{t}{\sqcup\!\sqcup} bv) + b(au \overset{t}{\sqcup\!\sqcup} v)) \\ &= R^t(a)S^t(u \overset{t}{\sqcup\!\sqcup} bv) + R^t(b)S^t(au \overset{t}{\sqcup\!\sqcup} v) \\ &= R^t(a)(S^t(u) \sqcup\!\sqcup S^t(bv)) + R^t(b)(S^t(au) \sqcup\!\sqcup S^t(bv)) \\ &= (R^t(a)S^t(u)) \sqcup\!\sqcup (R^t(b)S^t(v)) \\ &= S^t(w) \sqcup\!\sqcup S^t(w')\,, \end{aligned}$$

concluding the proof. □

Lemma 4.5.4. (⋆) The maps S^t and f commute.

Proof. Let S_0^t the restriction of S^t to $\mathfrak{h}^0[t]$, namely $S_0^t = S^t\big|_{\mathfrak{h}^0[t]} : \mathfrak{h}^0[t] \longrightarrow \mathfrak{h}^0[t]$. The map $S^t \circ f$ is a $*$-homomorphism by composition, satisfies the property $S^t \circ f(y) = S^t(0) = 0$, and extends the map S_0^t since

$$S^t \circ f(w) = S^t(w) = S_0^t(w)$$

for $w \in \mathfrak{h}^0[t]$. These three properties characterise it uniquely, for the same reason that f was characterised uniquely.

It remains only to show that $f \circ S^t$ also satisfies these properties. It is also a homomorphism by composition, satisfies $f \circ S^t(y) = f(y) = 0$ and extends S_0^t since

$$w \in \mathfrak{h}^0[t] \implies S^t(w) \in \mathfrak{h}^0[t] \implies f \circ S^t(w) = S^t(w) = S_0^t(w)\,.$$

By uniqueness, we conclude that $f \circ S^t = S^t \circ f$ as required. □

Theorem 4.5.3. (⋆) For all $w_0 \in \mathfrak{h}^0[t]$ and $w_1 \in \mathfrak{h}^1[t]$,

$$\zeta^t \circ f(w_0 \overset{t}{\sqcup\!\sqcup} w_1 - w_0 \overset{t}{*} w_1) = 0\,.$$

Proof. Recall that $\zeta^t = \zeta \circ S^t$. For all $w_0 \in \mathfrak{h}^0[t]$ and $w_1 \in \mathfrak{h}^1[t]$, we have

$$\begin{aligned} \zeta^t \circ f(w_0 \overset{t}{\sqcup\!\sqcup} w_1 - w_0 \overset{t}{*} w_1) &= \zeta \circ S^t \circ f(w_0 \overset{t}{\sqcup\!\sqcup} w_1 - w_0 \overset{t}{*} w_1) \\ &= \zeta \circ f \circ S^t(w_0 \overset{t}{\sqcup\!\sqcup} w_1 - w_0 \overset{t}{*} w_1) \\ &= \zeta \circ f(S^t(w_0) \sqcup\!\sqcup S^t(w_1) - S^t(w_0) * S^t(w_1))\,. \end{aligned}$$

Now $S^t(w_0) \in \mathfrak{h}^0[t]$ and $S^t(w_1) \in \mathfrak{h}^1[t]$, so the $\mathbb{Q}[t]$-linear extension of the EDS Theorem implies

$$\zeta^t \circ f(w_0 \overset{t}{\sqcup\!\sqcup} w_1 - w_0 \overset{t}{*} w_1) = 0\,.$$

□

Theorem 4.5.11. (⋆) The following equivalence holds:

$$\bar{D} = ker(\zeta) \iff \bar{D}^t = ker(\zeta^t)\,.$$

Proof. We prove the ($\Longrightarrow$) part and leave the other half as an exercise, which consists simply of replacing S^t by S^{-t} everywhere.

Assume $\bar{D} = ker(\zeta)$ and take an arbitrary element $w \in ker(\zeta^t)$. Then $\zeta^t(w) = \zeta(S^t(w)) = 0$, which implies that $S^t \in ker(\zeta)$. By assumption, this implies $S^t \in \bar{D}$ and so there exist $w_0 \in \mathfrak{h}^0$, $w_1 \in \mathfrak{h}^1$ such that

$$S^t(w) = f(w_0 \, ш \, w_1 - w_0 * w_1)\,.$$

Applying S^{-t} and using commutativity of S^t and f (lemma 4.5.5), this implies

$$w = f(S^{-t}(w_0 \, ш \, w_1) - S^{-t}(w_0 * w_1))\,.$$

Finally, theorems 4.3.5 and 4.4.6 imply that

$$w = f(S^{-t}(w_0) \overset{t}{ш} S^{-t}(w_1) - S^{-t}(w_0) \overset{t}{*} S^{-t}(w_1))\,,$$

which is by definition in $\bar{D}^t$ since $S^{-t}(\mathfrak{h}^0) \subset \mathfrak{h}^0$ and $S^{-t}(\mathfrak{h}^1) \subset \mathfrak{h}^1$. This proves that $\ker(\zeta^t) \subseteq \bar{D}^t$. The other containment $\bar{D}^t \subseteq ker(\zeta^t)$ holds by the t-EDS, so the proof is complete. □

A.5 Chapter 5

Proposition 5.3.7. ($\star$) The coproduct respects weight.

Proof. The coproduct is

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

so each (summed) term is of the form

$$I^{\mathfrak{m}}(a_0; a_{i_1}, \ldots, a_{i_k}; a_{n+1}) \otimes \prod_{p=0}^{k} I^{\mathfrak{m}}(a_{i_p}; a_{i_p+1}, \ldots, a_{i_{p+1}-1}; a_{i_{p+1}})$$

for some $0 \le k \le n$ and choice of indices $0 = i_0 < i_1 < \ldots < i_k < i_{k+1} = n+1$. Now

$$I^{\mathfrak{m}}(a_0; a_{i_1}, \ldots, a_{i_k}; a_{n+1})$$

has weight k and

$$I^{\mathfrak{m}}(a_{i_p}; a_{i_p+1}, \ldots, a_{i_{p+1}-1}; a_{i_{p+1}})$$

has weight $i_{p+1} - 1 - (i_p + 1) + 1 = i_{p+1} - i_p - 1$ for each $0 \le p \le k$. The sum telescopes, and it follows that the product

$$\prod_{p=0}^{k} I^{\mathfrak{m}}(a_{i_p}; a_{i_p+1}, \ldots, a_{i_{p+1}-1}; a_{i_{p+1}})$$

has weight

$$\sum_{p=0}^{k} i_{p+1} - i_p - 1 = i_{k+1} - i_0 - (k+1) = n - k\,.$$

Finally, the total weight of each term is

$$k + n - k = n$$

as claimed. □

Proof of Proposition 5.4.3. All proofs are my own unless stated otherwise.

R0: We have already proved **R0** when stating Goncharov's definition of motivic iterated integrals, which follows immediately from Kontsevich's formula.

R1: The first half of relation **R1** states that $I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) = 0$ for $n \geq 1$ and $a_0 = a_{n+1}$. We do not give a rigorous proof but this can be understood as the generalisation of the fact that integration from any point a to a in one variable is zero. The second half states that $I^{\mathfrak{m}}(a_0; \underbrace{a, \ldots, a}_{n}; a_{n+1}) = 0$ for any $n \geq 1$.

For $n = 1$, this holds by relation **R2**. For $n \geq 2$, we use induction and the shuffle product:

$$I^{\mathfrak{m}}(a_0; a; a_{n+1}) I^{\mathfrak{m}}(a_0; \underbrace{a, \ldots, a}_{n-1}; a_{n+1}) = 0 = I^{\mathfrak{m}}(a_0; \underbrace{a, \ldots, a}_{n}; a_{n+1})\,.$$

R2: Brown sets $I^{\mathfrak{m}}(a_0; a_1; a_2) = 0$ by definition. From my understanding, this holds because this object corresponds to an MZV of weight 1, but there are no such convergent MZVs. As such, we regularise this object by setting it to 0, somewhat like the 'filtering' function we introduced in Section 2.5 or like setting $\zeta(1) = 0$. Similarly, we set $I^{\mathfrak{m}}(a_0; a_1) = 1$ because this corresponds to an MZV of weight 0, so following our convention that $\zeta(\varnothing) = 1$ gives the above.

R3: This is proved in [Gon, Proposition 2.1].

R4: The statement is that $I^{\mathfrak{m}}(0; a_1, \ldots, a_n; 1) = I^{\mathfrak{m}}(0; 1 - a_n, \ldots, 1 - a_1; 1)$, which is exactly the duality theorem that we have proved for non-motivic MZVs. Note that $1 - a_i = \tau(a_i)$ for $a_i \in \{0, 1\}$, and the indices are swapped as in duality.

R5: the statement is that

$$(-1)^k I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n_1}, \ldots, \underbrace{0, \ldots, 0, 1}_{n_r}, \underbrace{0, \ldots, 0}_{k}; 1)$$

$$= \sum_{i_1 + \ldots + i_r = k} \binom{n_1 + i_1 - 1}{i_1} \cdots \binom{n_r + i_r - 1}{i_r} I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n_1 + i_1}, \ldots, \underbrace{0, \ldots, 0, 1}_{n_r + i_r}; 1)\,.$$

for any $k, n_1, \ldots, n_r \geq 1$. We prove this by induction on r. For $r = 1$, the claim is

$$(-1)^k I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n}, \underbrace{0, \ldots, 0}_{k}; 1) = \binom{n+k-1}{k} \zeta^{\mathfrak{m}}(n+k),$$

which is stated by Brown without proof in [Bro2, Eq. 4.10].

We prove this case by induction on k, extending to all $k \geq 0$ for convenience. The base case $k = 0$ is trivial since both sides are identical. Assume true for fixed $k \geq 0$ and all $n \geq 1$. By the shuffle relation,

$$\begin{aligned} I^{\mathfrak{m}}(0;0;1) I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n}, \underbrace{0, \ldots, 0}_{k}; 1) &= n I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n+1}, \underbrace{0, \ldots, 0}_{k}; 1) \\ &+ (k+1) I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n}, \underbrace{0, \ldots, 0}_{k+1}; 1). \end{aligned}$$

By **R2** the LHS is zero, and the inductive hypothesis gives

$$\begin{aligned} (-1)^{k+1} I^{\mathfrak{m}}(0; \underbrace{0, \ldots, 0, 1}_{n}, \underbrace{0, \ldots, 0}_{k+1}; 1) &= \frac{n}{k+1} \binom{n+k}{k} \zeta^{\mathfrak{m}}(n+1+k) \\ &= \frac{n}{k+1} \frac{(n+k) \ldots (n+1)}{k!} \zeta^{\mathfrak{m}}(n+k+1) \\ &= \binom{n+k}{k+1} \zeta^{\mathfrak{m}}(n+k+1) \end{aligned}$$

for all $n \geq 1$, as claimed. It remains only to perform the induction step on r. This is a more involved but purely combinatorial generalisation of the proof I have just given, which gives virtually no more insight into its meaning. We leave it as an exercise. □

Lemma 5.4.4. ($\star$) For any $n \in \mathbb{N}$,

$$\Delta \zeta(n) = \zeta(n) \otimes 1 + 1 \otimes \zeta(n).$$

Proof. By Goncharov's theorem,

$$\Delta \zeta^{\mathfrak{m}}(n) = -\Delta I^{\mathfrak{m}}(0; 0, \ldots, 0, 1; 1) =$$

$$- \sum_{0 = i_0 < i_1 < \ldots < i_k < i_{k+1} = n+1} I^{\mathfrak{m}}(0; a_{i_1}, \ldots, a_{i_k}; 1) \otimes \prod_{p=0}^{k} I^{\mathfrak{m}}(a_{i_p}; a_{i_p+1}, \ldots, a_{i_{p+1}-1}; a_{i_{p+1}}).$$

with $0 \leq k \leq n$. The terms corresponding to $k = 0$ and $k = n$ are

$$\zeta(n) \otimes 1 + 1 \otimes \zeta(n),$$

so it remains only to show that all other terms are zero. For $n = 1$ there are no other terms, so we are done. Otherwise, fix some $1 \leq k \leq n-1$. By relation (R2), each term

$$I^{\mathfrak{m}}(a_{i_p}; a_{i_p+1}, \ldots, a_{i_{p+1}-1}; a_{i_{p+1}})$$

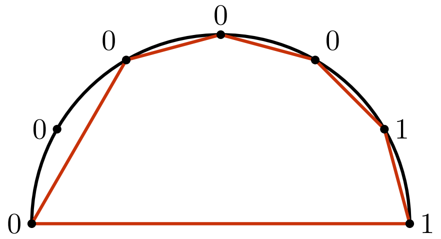
on the right-hand side is zero if $i_{p+1} - i_p > 1$ *and*

$$a_{i_p} = a_{i_{p+1}} \qquad or \qquad a_{i_p+1} = \ldots = a_{i_{p+1}-1} \, .$$

Now $\{i_1, \ldots, i_k\}$ is chosen as a subsequence of $\{1, \ldots, n\}$. If $i_k \neq n$ then $i_m < n$ for all $1 \leq m \leq k$, and since $a_j = 1$ only for $j = n$ or $j = n+1$, this implies $a_{i_m} = 0$ for all $1 \leq m \leq k$. Then the LHS of the tensor product is

$$I^{\mathfrak{m}}(0; a_{i_1}, \ldots, a_{i_k}; 1) = I^{\mathfrak{m}}(0; 0, \ldots, 0; 1) = 0 \, .$$

Now assume that $i_k = n$, and notice that $\{i_0, i_1, \ldots, i_k, i_{k+1}\}$ is a subsequence of $\{0, \ldots, n+1\}$. Since $k+1 \leq n$, at least one integer $1 \leq l \leq n-1$ is not chosen, so there is a 'gap' of at least 1 between some i_m. Visually speaking, this corresponds to the fact that any polygon



which is not the full or empty one, must have an edge which 'jumps' over some vertex a_m (here, $m = 1$).

More precisely, there exists $0 \leq m \leq k-1$ (which makes sense since $k \geq 1$) such that $i_{m+1} - i_m > 1$. Visually speaking, note that the 'jumping' edge in the polygon above must jump only over "0" vertices since the assumption $i_k = 1$ means that the k'th edge lands on the penultimate "1". The final "1" is always hit by definition, so neither cannot be jumped!

In technical terms: $m \leq k-1$ implies that $m+1 \leq k$, so the assumption $i_k = n$ gives $i_j < n$ for all $l < m+1$, and therefore $a_{i_j} = 0$ for all such j. Finally, taking the term $p = n$ in the product of the RHS gives

$$I^{\mathfrak{m}}(a_{i_m}; a_{i_m+1}, \ldots, a_{i_{m+1}-1}; a_{i_{m+1}}) = I^{\mathfrak{m}}(0; 0, \ldots, 0; a_{i_{m+1}}) = 0 \, .$$

We conclude that all terms with $1 \leq k \leq n-1$ are zero, and finally

$$\Delta \zeta^{\mathfrak{m}}(n) = \zeta(n) \otimes 1 + 1 \otimes \zeta(n) \, . \qquad \square$$

Appendix B

Algebraic background

For basic definitions of an algebra, bialgebra, coproduct, Hopf algebra, we refer to [Hen, Chapters 4,5].

B.1 Algebraic geometry

We define only the most elementary objects of affine algebraic geometry required for Chapter 5, following my notes on a course in algebraic curves. Let k a field, and

$$\mathbb{A}^n = \{(a_1, \ldots, a_n) \mid a_i \in K \text{ for all } i\}$$

the *affine n-space over k*. This is simply k^n as a set, but it is also a k-vector space and we follow this traditional notation. Take any set S of polynomials $f \in k[x_1, \ldots, x_n]$, and let

$$V(S) = \{x \in \mathbb{A}^n \mid f(x) = 0 \text{ for all } f \in S\},$$

the set of points in $\mathbb{A}^n$ for which all $f \in S$ vanish. Then $V(S)$ is called an *affine algebraic variety*. Now $V(S)$ could be generated by some other set of polynomials S', and it turns out that the variety is really determined by the *ideal* generated by the polynomials in S. Since the polynomial ring is Noetherian, every ideal is finitely generated and every affine algebraic variety can be generated by a finite set $S = \{f_1, \ldots, f_m\}$.

As such, we define a point $x \in V(S)$ to be *singular* if the Jacobian matrix J of first-order partial derivatives,

$$J_{ij} = \frac{\partial f_i}{\partial x_j},$$

has non-maximal rank at x. In other words, x is singular if there exists $y \in V(S)$ such that $\text{rank}(J(x)) < \text{rank}(J(y))$. For an algebraic variety defined by a single polynomial f, this condition is that x is singular if

$$\frac{\partial f}{\partial x_j}(x) = 0$$

for all $1 \leq j \leq n$. Then an affine algebraic variety V is called *smooth* if it contains no singular points.

B.2 Singular (co)homology

For any integer $n \geq 0$, define the standard n-simplex (of dimension n) by

$$\Delta^n = \{(t_0, \dots, t_n) \in \mathbb{R}^{n+1} \mid t_i \geq 0 \text{ and } \sum_{i=0}^{n} t_i = 1\}\,.$$

For each $0 \leq i \leq n$, Δ^n has a subset called a *face* which is homeomorphic to Δ^{n-1}. More precisely, there are homeomorphisms $\delta_i^n : \Delta^{n-1} \longrightarrow \Delta^n$ defined by

$$\delta_i^n(t_0, \dots, t_{n-1}) = (t_0, \dots, t_{i-1}, 0, t_i, \dots, t_{n-1})\,.$$

Given a topological space X, a singular n-simplex (or chain) is a continuous map $\sigma : \Delta^n \longrightarrow X$. We then define the *singular chain group* $C_n(X)$ (over $\mathbb{Z}$) to be the free abelian group generated by the singular n-chains,

$$C_n(X) = \bigoplus_{\sigma} \mathbb{Z}(\sigma)\,.$$

More precisely, elements of $C_n(X)$ are finite linear combinations

$$\sum_{i=1}^{r} a_i \sigma_i$$

with $a_i \in \mathbb{Z}$, σ_i singular n-chains. We then define the *boundary* map $d_n : C_n(X) \longrightarrow C_{n-1}(X)$, given on generators by its 'alternating decomposition' into faces,

$$d_n(\sigma) = \sum_{i=0}^{n} (-1)^i (\sigma \circ \delta_i^n)\,.$$

A simple exercise for the reader is to check that $d_n \circ d_{n+1} = 0$ for all $n \geq 0$, where we define $C_{-1}(X) = 0$ and thus $d_0 \equiv 0$ the zero map. We usually write this as $d^2 = 0$, omitting the subscripts, which turns $(C_*(X), d_*)$ into what we call a *chain complex*:

$$\dots \xrightarrow{d_{n+1}} C_n(X) \xrightarrow{d_n} \dots \xrightarrow{d_1} C_0(X) \xrightarrow{0} 0\,.$$

Note that the property $d^2 = 0$ implies $\operatorname{im}(d_{n+1}) \subseteq \ker(d_n)$ as groups. Finally, we define the singular homology groups of X as the group quotients

$$H_n(X) = \ker(d_n) / \operatorname{im}(d_{n+1})$$

for each $n \geq 0$. We call *cycles* elements in $\ker(d_n)$ (those in $H_n(X)$) and *boundaries* elements in $\operatorname{im}(d_{n+1})$ (those which are zero in $H_n(X)$). Note that a priori, the groups $C_*(X)$ may be immensely large (say uncountably infinite). It turns out that the groups $H_*(X)$ are relatively well-behaved because of the quotiented image, although may still be infinite.

A crucial theorem of algebraic topology states that if two topological spaces X, Y are homotopy equivalent, then their singular homology groups are isomorphic, $H_n(X) \cong H_n(Y)$ for all $n \geq 0$. As such, singular homology can be used to differentiate between topological spaces. Moreover, if two cycles σ_1, σ_2 in X are homotopic to each other, then $[\sigma_1] = [\sigma_2]$. This reinforces the idea that homology groups are much smaller, since 'most' of the cycles will be the same element in homology.

Example B.2.1. We follow [BGF, Example 2.3] in our own words, with much more detail. Let $M = \mathbb{C} \setminus \{0\}$ with the subspace topology induced from the usual (analytic) topology of $\mathbb{C}$, whose open sets are unions of balls

$$B_r^\epsilon = \{z \in \mathbb{C} \mid |z - r| < \epsilon\}$$

with $r \in \mathbb{C}$ the centre, $\epsilon > 0$ the radius. Now consider the singular chains $\sigma_0 : \Delta^0 \longrightarrow M$, $\sigma_1, \tau_1 : \Delta^1 \longrightarrow M$ and $\sigma_2 : \Delta^2 \longrightarrow M$ given by

$$\sigma_0(1) = 1\,,$$
$$\sigma_1(t, 1-t) = e^{2\pi i t}$$

whose images are the point $z = 1$ and the unit circle in $\mathbb{C} \setminus \{0\}$. Now any 0-simplex (point) in M is homotopic to σ_0 since it can be continuously deformed to the point 1. Similarly, any 1-simplex in M is homotopic to σ_1 since it can be continuously deformed to the unit circle. Now

$$\begin{aligned} d_1(\sigma_1)(1) &= \sigma_1 \circ \delta_0^1(1) - \sigma_1 \circ \delta_1^1(1) \\ &= \sigma_1(0,1) - \sigma_1(1,0) \\ &= e^0 - e^{2\pi i} \\ &= 0\,, \end{aligned}$$

so we obtain $d_1(\sigma_1) \equiv 0$ as a 0-simplex. It follows that $\sigma_1 \in \ker(d_1)$, i.e. $[\sigma_1] \in H_1(X)$. We leave it as a simple exercise for the reader to show that $[\sigma_1] \neq 0$, i.e. that there exists no $a \in C_2(M)$ such that $d_2(a) = \sigma_1$. [If there were, a would contain a 2-simplex whose interior contains $0 \in \mathbb{C}$, which is not in M]. By the remark above, the class of any other 1-simplex is equal to $[\sigma_1]$ in $H_1(M)$, so we $[\sigma_1]$ generates the first homology:

$$H_1(M) = \{a[\sigma_1] \mid a \in \mathbb{Z}\} = \mathbb{Z}([\sigma_1]) \cong \mathbb{Z}\,.$$

We will often abuse notation by writing

$$H_1(M) = \mathbb{Z}(\sigma_0)\,.$$

The zero'th homology is even simpler, since it is defined by

$$H_0(M) = \ker(d_0)/\operatorname{im}(d_1) = C_0/\operatorname{im}(d_1)\,.$$

Now σ_0 is not 0 in homology, since the boundary of any 1-simplex consists of two 0simplices, so taking any $c \in C_1$ will yield an even number of 0-simplices in $d(c)$, which cannot be equal to σ_0. Again, the remark above on homotopy gives us

$$H_0(M) = \mathbb{Z}(\sigma_0) \cong \mathbb{Z}\,.$$

The reader can check that all higher homology vanishes, so that

$$H_i(M) = \begin{cases} \mathbb{Z}(\sigma_0) & \text{if } i = 0 \\ \mathbb{Z}(\sigma_1) & \text{if } i = 1 \\ 0 & \text{else.} \end{cases}$$

We now turn to singular cohomology (over $\mathbb{Z}$). This is obtained by taking the dual groups of *singular co-chains*

$$C^n(X) = \operatorname{Hom}(C_n(X), \mathbb{Z}) = \{f : C_n(X) \longrightarrow \mathbb{Z} \mid f \text{ is continuous}\},$$

along with *coboundary* maps $\partial^n : C^n(X) \longrightarrow C^{n+1}(X)$ given by

$$\partial^n := d_{n+1}^{\#},$$

and the reader can check that $\partial^{n+1} \circ \partial^n = 0^* = 0$. The notation $\#$ is the standard dual one, defined as

$$d_{n+1}^{\#}(f)(\sigma) = f(d_{n+1}(\sigma))$$

for all $f \in C^n(X)$, $\sigma \in C_{n+1}(X)$. This makes sense since $d_{n+1} : C_{n+1}(X) \longrightarrow C_n(X)$. This again turns $(C^*(X), \partial^*)$ into a chain complex

$$\ldots \xleftarrow{\partial^n} C^n(X) \xleftarrow{\partial^{n-1}} \ldots \xleftarrow{\partial^0} C^0(X) \xleftarrow{0} 0.$$

As before, singular cohomology is defined by the homology of this new chain complex, or more precisely:

$$H^n(X) = \ker(\partial^n)/\operatorname{im}(\partial^{n-1})$$

for all $n \geq 0$.

Remark B.2.2. We have defined singular (co)homology with coefficients in $\mathbb{Z}$, but could have provided an identical construction with coefficients in another ring, say $\mathbb{Q}$. In the example for $M = \mathbb{C} \setminus \{0\}$, this would give exactly the same homology groups with $\mathbb{Z}$ replaced with $\mathbb{Q}$, which will be useful in Section 5.3.

We will not introduce relative (co)homology, as we will make the simplification of working without it throughout Chapter 5.

B.3 De Rham cohomology

As in the previous section, let X be a topological space. If X is moreover a differentiable manifold of dimension n, we can define a different type of cohomology named *de Rham*. The subject requires to introduce the (more sophisticated version) algebraic version of de Rham cohomology constructed by Gröthendieck, but this requires advanced knowledge of algebraic geometry beyond the scope of this report. As such, we give the original form given by de Rham, reproduced from a cross-section between [BGF, Sec. 2.2] and [BT, Chap. 1].

Define a differential p-form in the local coordinates $(x_1, \ldots, x_n)$ of X as

$$\omega = \sum_{1 \leq i_1 < \ldots < i_p \leq n} f_{i_1,\ldots,i_p}(x_1, \ldots, x_n) dx_{i_1} \wedge \ldots \wedge dx_{i_p},$$

where $f_{i_1,\ldots,i_p}$ is a smooth function. The wedge product $\wedge$ can simply be viewed as the usual product $\cdot$ along with extra information about the orientation of ambient space. The reader with no experience in differential geometry can take these as formal objects which we manipulate through certain axioms. Let $\Omega^p(X)$ the real vector space of such p-forms, and

$$\Omega(X) = \bigoplus_{p=0}^{n} \Omega^p(X)\,.$$

Define the *exterior derivative* $d : E(X) \longrightarrow E(X)$ as the unique $\mathbb{R}$-linear map sending p-forms to $(p+1)$-forms satisfying the following properties.

(1) If f is a smooth function then df is the *differential* of f.

(2) $d^2 = 0$.

(3) $d(\alpha \wedge \beta) = (d\alpha) \wedge \beta + (-1)^p \alpha \wedge (d\beta)$ for any $\alpha \in \Omega^p(X)$ and $\beta \in \Omega(X)$.

Note that the differential of a smooth function f is the generalisation of 'total derivatives' to differentiable manifolds. In local coordinates $(x_1, \ldots, x_n)$, the differential is given by

$$df = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} dx_i\,.$$

To be more precise, we deduce from these axioms that for any p-form ω we obtain

$$\begin{aligned}
d\omega &= d(f dx_{i_1} \wedge \ldots \wedge dx_{i_p} \\
&= df \wedge (dx_{i_1} \wedge \ldots \wedge dx_{i_p}) + (-1)^0 f d(dx_{i_1} \wedge \ldots \wedge dx_{i_p}) \\
&= df \wedge dx_{i_1} \wedge \ldots \wedge dx_{i_p} \\
&= \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} dx_i \wedge dx_{i_1} \wedge \ldots \wedge dx_{i_p}\,,
\end{aligned}$$

where $(-1)^0$ appears because f is a 0-form, and the second term vanishes since expanding gives only $d^2 = 0$ terms. Before moving on, we define a differential form ω to be *closed* if $d\omega = 0$.

Since d sends p-forms to $(p+1)$-forms, we can also decompose d into maps $d^p : \Omega^p(X) \longrightarrow \Omega^{p+1}(X)$, reminding us of singular cohomology. Since these maps satisfy $d^2 = 0$, we obtain a chain complex

$$0 \xleftarrow{0} \Omega^n(X) \xleftarrow{d^{n-1}} \ldots \xleftarrow{d^0} \Omega^0(X) \xleftarrow{0} 0$$

whose homology $H^p_{\mathrm{dR}}(X)$ is the *de Rham cohomology* of X. More precisely,

$$H^p_{\mathrm{dR}}(X) \coloneqq \ker(d^p)/\operatorname{im}(d^{p-1})$$

for all $0 \leq p \leq n$.

Remark B.3.1. The algebraic version of de Rham cohomology allows us to perform the above construction for any affine algebraic variety X over a field of characteristic zero k, which is not necessarily a differentiable manifold. Moreover, it suffices in this case "to consider differential forms with polynomial coefficients" rather than any smooth function f. In the example below, we take $k = \mathbb{Q}$.

Example B.3.2. We follow [BGF, Example 2.25] in our own words, with much more detail. Let X the affine variety given by the polynomial $f(x,y) = xy - 1 \in \mathbb{Q}[x,y]$. For the reader with no knowledge of algebraic variety, M is explicitly given by the set

$$X = \{(x,y) \in \mathbb{Q}^2 \mid f(x,y) = 0\} = \{(x, 1/x) \mid x \in \mathbb{Q} \setminus \{0\}\} \cong \mathbb{Q} \setminus \{0\}\,.$$

Note that the set of complex points $M := X(\mathbb{C})$, the set of solutions to $f = 0$ with coordinates in $\mathbb{C}$, is

$$M = \{(x, 1/x) \mid x \in \mathbb{C} \setminus \{0\}\} \cong \mathbb{C} \setminus \{0\}\,,$$

which is the space considered in B.2.1. Now M is a differentiable manifold but X itself is *not*, but the remark above allows us to compute its algebraic de Rham cohomology without details of its construction. Moreover, we can consider differential forms with polynomial coefficients only. Now we must keep in mind that $y = 1/x$, so p-differential forms on X are generated as rational vector spaces by

$$\omega = x^n y^m = x^{n-m}$$

for $p = 0$ and

$$\omega = x^n y^m dx = x^{n-m} dx$$

for $p = 1$, where $n, m \in \mathbb{N} \cup \{0\}$. Note that there are no 2-forms since

$$dx \wedge dy = \frac{-1}{x^2} dx \wedge dx = 0$$

by antisymmetry of the wedge product. To summarise, p-differential forms on X are generated by

$$\omega = x^n \qquad \text{and} \qquad \omega = x^n dx$$

for $p = 0, 1$ respectively, where $n \in \mathbb{N} \cup \{0\}$. The exterior derivative $d : E(X) \longrightarrow E(X)$ is given by

$$d^0(x^n) = n x^{n-1} dx$$

for $p = 0$ and

$$d^1(x^n dx) = 0$$

for $p = 1$, since d^1 sends 1-forms to 2-forms, but there are none of the latter. Now $d_0(x^n)$ only vanishes for $n = 0$, so the zero'th cohomology group is

$$H^0_{\mathrm{dR}}(X) = \ker(d_0) = \mathrm{span}_{\mathbb{Q}}\{x^0\} = \mathbb{Q}\,.$$

For the first cohomology, we have

$$\ker(d_1) = \Omega^1(X) = \mathrm{span}_{\mathbb{Q}}\{x^n dx\}$$

and

$$\mathrm{im}(d_0) = \mathrm{span}_{\mathbb{Q}}\{x^n dx \mid n \neq -1\}\,.$$

This holds because $d_0(\frac{x^{n+1}}{n+1}) = x^n dx$ for all $n \neq -1$, but we cannot attain the case $n = -1$ since the antiderivative of $1/x$ is $log(x)$, which is absent from our vector space. Finally, we obtain

$$H^1_{\mathrm{dR}}(X) = \ker(d_1)/\,\mathrm{im}(d_0) = \mathrm{span}_{\mathbb{Q}}\{x^{-1} dx\} = \mathbb{Q}\left(\frac{dx}{x}\right)\,.$$

The higher cohomologies all vanish trivially.