# On the decomposition of motivic multiple zeta values 

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#### Abstract

. We review motivic aspects of multiple zeta values, and as an application, we give an exact-numerical algorithm to decompose any (motivic) multiple zeta value of given weight into a chosen basis up to that weight.


## §1. Introduction

The aim of these notes is to present motivic aspects of multiple zeta values in concrete terms, and give applications which might be of use to physicists. Most introductory texts on multiple zeta values focus exclusively on the many relations they are known to satisfy. Here we take a very different approach. The general philosophy of motives suggests that classical Galois theory should extend to certain families of transcendental numbers (namely periods). Multiple zeta values would be a prototypical example in such a Galois theory. But since the transcendence conjectures for multiple zeta values are completely unknown, such a theory is at present totally inaccessible. One way to circumvent this is to replace multiple zeta values with more abstractly defined objects called motivic multiple zeta values, for which such a Galois action makes sense. Concretely, this takes the form of a coalgebra structure underlying the motivic multiple zeta values. One of the purposes of this paper is to show how one can do effective Galois-theoretic calculations with motivic multiple zeta values and use this to deduce new results about actual multiple zeta values. There are two applications:
(1) we show how to use the coalgebra structure to decompose any multiple zeta value numerically into a candidate basis.

[^0](2) we show how to lift certain identities between multiple zeta values, i.e., real numbers, to their motivic versions.
The first point requires explanation. Since the $\mathbb{Q}$-vector space of multiple zeta values is finite-dimensional in each weight, standard lattice reduction algorithms give a numerical way to write an arbitrary multiple zeta value of given weight in terms of some chosen spanning set. The point of (1) is that the coalgebra structure enables one to replace this single high-dimensional lattice reduction problem with a sequence of one-dimensional lattice reductions. This is simply the problem of identifying a rational number $\alpha \in \mathbb{Q}$ which is presented as an element $\alpha \in \mathbb{R}$ to arbitrarily high accuracy, and can be done using continued fractions. In fact, we expect that there exists a relatively small a priori bound on the denominators of the rational numbers $\alpha$ which can arise, and so this algorithm is efficient in practice.

An application of (2) might be to prove that certain families of relations between multiple zeta values are 'motivic'. The idea behind this was used for the main theorem of [1], where one had to lift some relations between actual multiple zeta values to their motivic versions.

The paper is set out as follows. In $\S 2$, we review some basic properties of iterated integrals for motivation. In $\S 3$ we briefly review the structure of the category of mixed Tate motives over $\mathbb{Z}$ and state the main properties of motivic multiple zeta values. In $\S 4$ we show how to define derivation operators $\partial_{2 k+1}^{\phi}$, where $k \geq 1$, which act on the space of motivic multiple zeta values, and encode the action of the motivic Galois Lie algebra. In $\S 5$ we describe the decomposition algorithm (1) using these operators, and in $\S 6$ we provide a worked example of this algorithm. The reader who is only interested in implementing the algorithm may turn immediately to $\S \S 5.1-5.2$, which can be read independently from the rest of the paper.

## §2. Iterated Integrals

We begin with some generalities on iterated integrals, before specializing to the case of iterated integrals on the punctured projective line.

### 2.1. General iterated integrals

Let $M$ be a smooth $C^{\infty}$ manifold over $\mathbb{R}$, and let $k$ be the real or complex numbers. Let $\gamma:[0,1] \rightarrow M$ be a piecewise smooth path on $M$, and let $\omega_{1}, \ldots, \omega_{n}$ be smooth $k$-valued 1-forms on $M$. Let us write

$$
\gamma^{*}\left(\omega_{i}\right)=f_{i}(t) d t
$$

for the pull-back of the forms $\omega_{i}$ to the interval $[0,1]$.
Definition 2.1. Let the iterated integral of $\omega_{1}, \ldots, \omega_{n}$ along $\gamma$ be

$$
\begin{equation*}
\int_{\gamma} \omega_{1} \ldots \omega_{n}=\int_{0 \leq t_{1} \leq \ldots \leq t_{n} \leq 1} f_{1}\left(t_{1}\right) d t_{1} \ldots f_{n}\left(t_{n}\right) d t_{n} \tag{2.1}
\end{equation*}
$$

More generally, an iterated integral is any $k$-linear combination of such integrals. The empty integral $(n=0)$ is defined to be the constant 1 .

The iterated integrals $\int_{\gamma} \omega_{1} \ldots \omega_{n}$ do not depend on the choice of parametrization of the path $\gamma$, and satisfy the following basic properties:

Shuffle product formula. Given 1-forms $\omega_{1}, \ldots, \omega_{r+s}$ one has:

$$
\int_{\gamma} \omega_{1} \ldots \omega_{r} \int_{\gamma} \omega_{r+1} \ldots \omega_{r+s}=\sum_{\sigma \in \Sigma(r, s)} \int_{\gamma} \omega_{\sigma(1)} \ldots \omega_{\sigma(n)}
$$

where $n=r+s$, and $\Sigma(r, s)$ is the set of $(r, s)$-shuffles:

$$
\begin{aligned}
\Sigma(r, s)=\left\{\sigma \in \Sigma(n): \sigma^{-1}(1)<\right. & \ldots<\sigma^{-1}(r) \\
& \text { and } \left.\sigma^{-1}(r+1)<\ldots<\sigma^{-1}(r+s)\right\} .
\end{aligned}
$$

As a general rule, for any letters $a_{1}, \ldots, a_{r+s}$, we shall formally write

$$
\begin{equation*}
a_{1} \ldots a_{r} \amalg a_{r+1} \ldots a_{r+s}=\sum_{\sigma \in \Sigma(r, s)} a_{\sigma(1)} \ldots a_{\sigma(r+s)} \tag{2.2}
\end{equation*}
$$

viewed in $\mathbb{Z}\left\langle a_{1}, \ldots, a_{r+s}\right\rangle$, the free $\mathbb{Z}$-module spanned by words in the $a$ 's.

Composition of paths. If $\alpha, \beta: I \rightarrow M$ are two piecewise smooth paths such that $\beta(0)=\alpha(1)$, then let $\alpha \beta$ denote the composed path obtained by traversing first $\alpha$ and then $\beta$. Then

$$
\int_{\alpha \beta} \omega_{1} \ldots \omega_{n}=\sum_{i=0}^{n} \int_{\alpha} \omega_{1} \ldots \omega_{i} \int_{\beta} \omega_{i+1} \ldots \omega_{n}
$$

where recall that the empty iterated integral $(n=0)$ is the constant 1 .
Reversal of paths. If $\gamma^{-1}(t)=\gamma(1-t)$ denotes the reversal of the path $\gamma$, then we have the following reflection formula:

$$
\int_{\gamma^{-1}} \omega_{1} \ldots \omega_{n}=(-1)^{n} \int_{\gamma} \omega_{n} \ldots \omega_{1}
$$

Functoriality. If $f: M^{\prime} \rightarrow M$ is a smooth map, and $\gamma:[0,1] \rightarrow M^{\prime}$ a piecewise smooth path, then we have:

$$
\int_{\gamma} f^{*} \omega_{1} \ldots f^{*} \omega_{n}=\int_{f(\gamma)} \omega_{1} \ldots \omega_{n}
$$

### 2.2. The punctured projective line

Now let us consider the case where $k=\mathbb{C}, S$ is a finite set of points in $\mathbb{C}$, and $M=\mathbb{C} \backslash S$. Consider the set of closed one forms

$$
\begin{equation*}
\frac{d z}{z-a_{i}} \in \Omega^{1}(M) \text { where } a_{i} \in S \tag{2.3}
\end{equation*}
$$

Let $a_{0}, a_{n+1} \in M$ and let $\gamma$ be a path with endpoints $\gamma(0)=a_{0}, \gamma(1)=$ $a_{n+1}$. Using the notation from [5], set:

$$
\begin{equation*}
I_{\gamma}\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)=\int_{\gamma} \frac{d z}{z-a_{1}} \ldots \frac{d z}{z-a_{n}} \tag{2.4}
\end{equation*}
$$

Since the exterior product of any two forms (2.3) is zero and each one is closed, one can show that the iterated integrals (2.4) only depend on the homotopy class of $\gamma$ relative to its endpoints. When the path $\gamma$ is clear from the context, it can be dropped from the notation.

A variant is to take the limit points $a_{0}, a_{n+1}$ in the set $S$, in which case only the interior of $\gamma([0,1])$ lies in $M$. When the integral (2.4) converges, we can extend the definition to this case and show that the basic properties of $\S 2.1$ still hold. Even when it does not converge, (2.4) can be defined by a suitable logarithmic regularization procedure (tangential basepoint).

### 2.3. Multiple zeta values

From now on, we shall only consider the case where $M=\mathbb{C} \backslash\{0,1\}$, and thus all $a_{i} \in\{0,1\}$. There is a canonical path $\gamma:(0,1) \rightarrow M$ where $\gamma(t)=t$, but note that the endpoints of $\gamma$ no longer lie in $M$. Write

$$
\begin{align*}
\rho: \mathbb{N}_{+}^{r} & \longrightarrow\{0,1\}^{\times}  \tag{2.5}\\
\rho\left(n_{1}, \ldots, n_{r}\right) & =10^{n_{1}-1} \ldots 10^{n_{r}-1}
\end{align*}
$$

where $0^{k}$ denotes a sequence of $k$ zeros, and $\mathbb{N}_{+}=\mathbb{N} \backslash\{0\}$. When $n_{r} \geq 2$, the following iterated integral and sum converge absolutely, and we have

$$
\begin{align*}
I_{\gamma}\left(0 ; \rho\left(n_{1}, \ldots, n_{r}\right) ; 1\right) & =(-1)^{r} \sum_{0<k_{1}<\ldots<k_{r}} \frac{1}{k_{1}^{n_{1} \ldots k_{r}^{n_{r}}}}  \tag{2.6}\\
& =(-1)^{r} \zeta\left(n_{1}, \ldots, n_{r}\right)
\end{align*}
$$

This is easily verified from a geometric expansion of $\frac{d t}{t-1}$. In this case, the word $\rho\left(n_{1}, \ldots, n_{r}\right) \in\{0,1\}^{\times}$begins in 1 and ends in 0 , and is called a convergent word in 0,1 for obvious reasons. In general, for any sequence $\left(n_{1}, \ldots, n_{r}\right) \in \mathbb{N}_{+}^{r}$, the quantity $\sum_{i} n_{i}$ is called the weight, and $r$ the depth.

Note that the sign conventions in this paper are the usual ones, and differ from those in [1].

### 2.4. Regularization of MZV's

One can extend the definition of $I_{\gamma}\left(0 ; a_{1}, \ldots, a_{n} ; 1\right)$ with $a_{i} \in\{0,1\}$ from the set of convergent words to the general case by using the shuffle product formula. We henceforth drop the $\gamma$ from the subscript.

Lemma 2.2. There is a unique way to define a set of real numbers $I\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)$ for any $a_{i} \in\{0,1\}$, such that

- $I\left(0 ; a_{1}, \ldots, a_{n} ; 1\right)$ is given by (2.6) if $a_{1}=1$ and $a_{n}=0$.
- $I\left(a_{0} ; a_{1} ; a_{2}\right)=0$ and $I\left(a_{0} ; a_{1}\right)=1$ for all $a_{0}, a_{1}, a_{2} \in\{0,1\}$.
- (Shuffle product). For all $n=r+s$ and $a_{0}, \ldots, a_{n+1} \in\{0,1\}$

$$
\begin{array}{r}
I\left(a_{0} ; a_{1}, \ldots, a_{r} ; a_{n+1}\right) I\left(a_{0} ; a_{r+1}, \ldots, a_{r+s} ; a_{n+1}\right) \\
\quad=\sum_{\sigma \in \Sigma(r, s)} I\left(a_{0} ; a_{\sigma(1)}, \ldots, a_{\sigma(r+s)} ; a_{n+1}\right)
\end{array}
$$

- $\quad I\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)=0$ if $a_{0}=a_{n+1}$ and $n \geq 1$.
- $I\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)=(-1)^{n} I\left(a_{n+1} ; a_{n}, \ldots, a_{1} ; a_{0}\right)$.
- $I\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)=(-1)^{n} I\left(1-a_{n+1} ; 1-a_{n}, \ldots ; 1-a_{0}\right)$.

In particular, every iterated integral $I\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)$ is a linear combination of multiple zeta values $\zeta\left(n_{1}, \ldots, n_{r}\right)$ with $n_{i} \geq 1$ and $n_{r} \geq 2$.

The second last equation is simply the reversal of paths formula, the last equation is functoriality with respect to the map $t \mapsto 1-t$. The numbers $\zeta\left(n_{1}, \ldots, n_{r}\right)$ defined for any $n_{i} \in \mathbb{N}_{+}$by $(-1)^{r} I\left(0 ; \rho\left(n_{1}, \ldots, n_{r}\right) ; 1\right)$ are sometimes called shuffle-regularized multiple zeta values.

### 2.5. Structure of MZV's in low weights

Let $\mathcal{Z}_{N}$ denote the $\mathbb{Q}$-vector space spanned by the set of multiple zeta values $\zeta\left(n_{1}, \ldots, n_{r}\right)$ with $n_{r} \geq 2$ of total weight $N=n_{1}+\ldots+n_{r}$, and let $\mathcal{Z}$ denote the $\mathbb{Q}$-algebra spanned by all multiple zeta values over $\mathbb{Q}$. It is the sum of the vector spaces $\mathcal{Z}_{N} \subset \mathbb{R}$, and conjecturally a direct sum. By standard lattice reduction methods, one can try to write down a conjectural basis for $\mathcal{Z}$ for weight $\leq N$. Up to weight 10 , one experimentally obtains:

| Weight $N$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathcal{Z}_{N}$ | $\emptyset$ | $\zeta(2)$ | $\zeta(3)$ | $\zeta(2)^{2}$ | $\zeta(5)$ <br> $\zeta(3) \zeta(2)$ | $\zeta(3)^{2}$ <br> $\zeta(2)^{3}$ | $\zeta(7)$ <br> $\zeta(5) \zeta(2)$ <br> $\zeta(3) \zeta(2)^{2}$ | $\zeta(3,5)$ <br> $\zeta(3) \zeta(5)$ <br> $\zeta(3)^{2} \zeta(2)$ <br> $\zeta(2)^{4}$ |
|  |  |  |  |  |  |  |  | 4 |
| $\operatorname{dim}_{\mathbb{Q}} \mathcal{Z}_{N}$ | 0 | 1 | 1 | 1 | 2 | 2 | 3 | 4 |


| Weight $N$ | 9 | 10 |
| :---: | :---: | :---: |
| $\mathcal{Z}_{N}$ | $\zeta(9)$ | $\zeta(3,7)$ |
|  | $\zeta(3)^{3}$ | $\zeta(3) \zeta(7)$ |
|  | $\zeta(7) \zeta(2)$ | $\zeta(5)^{2}$ |
|  | $\zeta(5) \zeta(2)^{2}$ | $\zeta(3,5) \zeta(2)$ |
|  | $\zeta(3) \zeta(2)^{3}$ | $\zeta(3) \zeta(5) \zeta(2)$ |
|  |  | $\zeta(3)^{2} \zeta(2)^{2}$ |
|  |  | $\zeta(2)^{5}$ |
| $\operatorname{dim}_{\mathbb{Q}} \mathcal{Z}_{N}$ | 5 | 7 |

The dimensions at the bottom are conjectural, and it is not even known whether $\zeta(5)$ and $\zeta(3) \zeta(2)$ are linearly independent over $\mathbb{Q}$.

For example, the table implies that there exists a relation between the two multiple zeta values $\zeta(3)$ and $\zeta(1,2)$ in weight 3 , and indeed it was shown by Euler that $\zeta(3)=\zeta(1,2)$. In weight 8 there appears the first multiple zeta value $\zeta(3,5)$ which conjecturally cannot be expressed as a polynomial in the single zetas $\zeta(n)$ with coefficients in $\mathbb{Q}$. One expects

$$
\{\zeta(2), \zeta(3), \zeta(5), \zeta(7), \zeta(3,5), \zeta(9), \zeta(3,7)\}
$$

to be algebraically independent over $\mathbb{Q}$.

## §3. Motivic formalism

### 3.1. The category of mixed Tate motives over $\mathbb{Z}$

Let $\mathcal{M T}(\mathbb{Z})$ denote the category of mixed Tate motives over $\mathbb{Z}[4]$. This is a Tannakian category whose simple objects are the Tate motives $\mathbb{Q}(n)$, indexed by $n \in \mathbb{Z}$, and which have weight $-2 n$. The structure of $\mathcal{M} \mathcal{T}(\mathbb{Z})$ is determined by the data:

$$
\operatorname{Ext}_{\mathcal{M} \mathcal{T}(\mathbb{Z})}^{1}(\mathbb{Q}(0), \mathbb{Q}(n)) \cong \begin{cases}\mathbb{Q} & \text { if } n \geq 3 \text { is odd }  \tag{3.1}\\ 0 & \text { otherwise }\end{cases}
$$

and the fact that the $\operatorname{Ext}^{2}$ 's vanish. Thus $\mathcal{M} \mathcal{T}(\mathbb{Z})$ is equivalent to the category of representations of an affine group scheme $\mathcal{G}_{\mathcal{M T}}$ over $\mathbb{Q}$, which is a semi-direct product

$$
\begin{equation*}
\mathcal{G}_{\mathcal{M T}} \cong \mathcal{G}_{\mathcal{U}} \rtimes \mathbb{G}_{m} \tag{3.2}
\end{equation*}
$$

where $\mathcal{G}_{\mathcal{U}}$ is the prounipotent algebraic group over $\mathbb{Q}$ whose Lie algebra is the free Lie algebra with one generator $\sigma_{2 n+1}$ in degree $-(2 n+1)$ for all $n \geq 1$. The generators correspond to (3.1), and the freeness follows from the vanishing of the Ext ${ }^{2}$ 's. The motivic weight is twice the degree.

Remark 3.1. Henceforth we shall use the word weight to refer to half the motivic weight, in keeping with the usual terminology for MZV's.

Definition 3.2. Let $\mathcal{A}^{\mathcal{M} \mathcal{T}}$ denote the graded ring of affine functions on $\mathcal{G}_{\mathcal{U}}$ over $\mathbb{Q}$. It is a commutative graded Hopf algebra whose coproduct we denote by

$$
\Delta: \mathcal{A}^{\mathcal{M} \mathcal{T}} \longrightarrow \mathcal{A}^{\mathcal{M} \mathcal{T}} \otimes_{\mathbb{Q}} \mathcal{A}^{\mathcal{M} \mathcal{T}}
$$

Define a graded algebra-comodule over $\mathcal{A}^{\mathcal{M T}}$ by:

$$
\begin{equation*}
\mathcal{H}^{\mathcal{M} \mathcal{T}_{+}}=\mathcal{A}^{\mathcal{M} \mathcal{T}} \otimes_{\mathbb{Q}} \mathbb{Q}\left[f_{2}\right] \tag{3.3}
\end{equation*}
$$

where $f_{2}$ is defined to be of degree 2 and has trivial coaction. The map $\mathcal{H}^{\mathcal{M} \mathcal{T}_{+}} \rightarrow \mathcal{A}^{\mathcal{M} \mathcal{T}}$ sends $f_{2}$ to 0 . As a graded vector space,

$$
\mathcal{H}^{\mathcal{M} \mathcal{T}_{+}} \cong \bigoplus_{k \geq 0} \mathcal{A}^{\mathcal{M} \mathcal{T}}[2 k]
$$

where $[2 k]$ denotes a shift in degree of $+2 k$. We also write the coaction:

$$
\Delta: \mathcal{H}^{\mathcal{M} \mathcal{T}_{+}} \longrightarrow \mathcal{A}^{\mathcal{M T}} \otimes_{\mathbb{Q}} \mathcal{H}^{\mathcal{M} \mathcal{T}_{+}}
$$

It is determined by (3.3) and the formula $\Delta\left(f_{2}\right)=1 \otimes f_{2}$.
The structure of $\mathcal{H}^{\mathcal{M} \mathcal{T}}+$ can be described explicitly as follows. It follows from the remarks above that $\mathcal{A}^{\mathcal{M T}}$ is non-canonically isomorphic to the cofree Hopf algebra on cogenerators $f_{2 r+1}$ in degree $2 r+1 \geq 3$ :

$$
\mathcal{U}^{\prime}=\mathbb{Q}\left\langle f_{3}, f_{5}, \ldots\right\rangle
$$

This has a basis consisting of all non-commutative words in the $f_{\text {odd }}$ 's. The notation $\mathcal{U}^{\prime}$ is superfluous but useful since we will need to consider many different isomorphisms $\mathcal{A}^{\mathcal{M} \mathcal{T}} \cong \mathcal{U}^{\prime}$. Again, we denote the coproduct on $\mathcal{U}^{\prime}$ by $\Delta$ (no confusion arises in practice, since the coproducts on $\mathcal{A}^{\mathcal{M T}}$ and $\mathcal{U}^{\prime}$ are compatible). It is given by deconcatenation:

$$
\begin{align*}
\Delta: \mathcal{U}^{\prime} \longrightarrow & \mathcal{U}^{\prime} \otimes \mathbb{Q} \mathcal{U}^{\prime}  \tag{3.4}\\
\Delta\left(f_{i_{1}} \ldots f_{i_{r}}\right) & =1 \otimes f_{i_{1}} \ldots f_{i_{r}}+f_{i_{1}} \ldots f_{i_{r}} \otimes 1 \\
& +\sum_{k=1}^{r-1} f_{i_{1}} \ldots f_{i_{k}} \otimes f_{i_{k+1}} \ldots f_{i_{r}} .
\end{align*}
$$

The multiplication on $\mathcal{U}^{\prime}$ is given by the shuffle product (2.2).
By analogy with $\mathcal{H}^{\mathcal{M}} \mathcal{T}_{+}$let us define a trivial algebra-comodule

$$
\mathcal{U}=\mathcal{U}^{\prime} \otimes_{\mathbb{Q}} \mathbb{Q}\left[f_{2}\right]=\mathbb{Q}\left\langle f_{3}, f_{5}, \ldots\right\rangle \otimes_{\mathbb{Q}} \mathbb{Q}\left[f_{2}\right]
$$

where $f_{2}$ is of degree 2 and commutes with the $f_{\text {odd }}$. The coaction

$$
\Delta: \mathcal{U} \longrightarrow \mathcal{U}^{\prime} \otimes_{\mathbb{Q}} \mathcal{U}
$$

satisfies $\Delta\left(f_{2}\right)=1 \otimes f_{2}$. The total degree gives a grading $\mathcal{U}_{k}$ on $\mathcal{U}$ which we call the weight (Remark 3.1).

Thus we have a non-canonical isomorphism

$$
\begin{equation*}
\psi: \mathcal{H}^{\mathcal{M} \mathcal{T}_{+}} \cong \mathcal{U} \tag{3.5}
\end{equation*}
$$

of graded algebra-comodules, which induces an isomorphism of the underlying graded Hopf algebras $\mathcal{A}^{\mathcal{M} \mathcal{T}}$ and $\mathcal{U}^{\prime}$, and maps $f_{2}$ to $f_{2}$.

Lemma 3.3. Let $d_{k}=\operatorname{dim} \mathcal{U}_{k}=\operatorname{dim} \mathcal{H}_{k}^{\mathcal{M} \mathcal{T}_{+}}$. Then

$$
\begin{equation*}
\sum_{k \geq 1} d_{k} t^{k}=\frac{1}{1-t^{2}-t^{3}} \tag{3.6}
\end{equation*}
$$

In particular, $d_{0}=1, d_{1}=0, d_{2}=1$ and $d_{k}=d_{k-2}+d_{k-3}$ for $k \geq 3$.
Proof. The Poincaré series of $\mathbb{Q}\left\langle f_{3}, f_{5}, \ldots\right\rangle$ is given by

$$
\frac{1}{1-t^{3}-t^{5}-\ldots}=\frac{1-t^{2}}{1-t^{2}-t^{3}}
$$

Multiplying by the Poincaré series $\frac{1}{1-t^{2}}$ for $\mathbb{Q}\left[f_{2}\right]$ gives (3.6). $\quad$ Q.E.D.
If we define the depth of $f_{2 i+1}$ to be 1 for all $i>0$, and the depth of $f_{2}$ to be 0 , then we obtain a grading on $\mathcal{U}$ which simply counts the number of odd elements $f_{2 i+1}$. The motivic depth is the associated increasing filtration and can be defined in terms of the coaction $\mathcal{H}^{\mathcal{M} \mathcal{T}_{+}} \rightarrow \mathcal{A}^{\mathcal{M T}} \otimes_{\mathbb{Q}} \mathcal{H}^{\mathcal{M} \mathcal{T}_{+}}$. One checks that the motivic depth filtration induced on $\mathcal{H}^{\mathcal{M}} \mathcal{T}_{+}$by (3.5) is well-defined, and independent of the choice of $\psi$. In other words, the depth filtration is motivic, but the depth grading is not. This stems from the fact that $\sigma_{2 i+1}$ is well-defined only up to addition of commutators of $\sigma_{j}$ for $j<2 i+1$.

Example 3.4. Compare the structure of $\mathcal{H}^{\mathcal{M}}{ }_{+}$in low weights with the table of multiple zeta values given in $\S 2.5$ :

| Weight $k$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Basis for $\mathcal{H}_{k}^{\mathcal{M} \mathcal{T}}+$ | $\emptyset$ | $f_{2}$ | $f_{3}$ | $f_{2}^{2}$ | $\begin{gathered} f_{5} \\ f_{3} f_{2} \end{gathered}$ | $f_{3} \underset{f_{2}^{3}}{ } f_{3}$ | $\begin{gathered} f_{7} \\ f_{5} f_{2} \\ f_{3} f_{2}^{2} \end{gathered}$ | $\begin{gathered} f_{5} f_{3} \\ f_{3} \amalg f_{5} \\ f_{3} \amalg f_{3} f_{2} \\ f_{2}^{4} \end{gathered}$ | $\begin{gathered} f_{9} \\ f_{3} \amalg f_{3} \amalg f_{3} \\ f_{7} f_{2} \\ f_{5} f_{2}^{2} \\ f_{3} f_{2}^{3} \end{gathered}$ | $\begin{gathered} f_{7} f_{3} \\ f_{3} \text { W } f_{7} \\ f_{5} \text { III } f_{5} \\ f_{5} f_{3} f_{2} \\ f_{3} \amalg f_{5} f_{2} \\ f_{3} \amalg f_{3} f_{2}^{2} \\ f_{2}^{5} \\ \hline \end{gathered}$ |
| dim | 0 | 1 | 1 | 1 | 2 | 2 | 3 | 4 | 5 | 7 |

The following well-known conjecture is of a transcendental nature.
Conjecture 1. The $\mathbb{Q}$-algebra of MZV's is graded by the weight:

$$
\begin{equation*}
\mathcal{Z} \cong \bigoplus_{k \geq 0} \mathcal{Z}_{k} \tag{3.7}
\end{equation*}
$$

and there is an isomorphism of graded algebras:

$$
\begin{equation*}
\mathcal{Z} \cong \mathcal{H}^{\mathcal{M} \mathcal{T}_{+}} \tag{3.8}
\end{equation*}
$$

The first part (3.7) implies that there should be no relations between multiple zeta values of different weights. The second (3.8) implies in particular that the multiple zeta values should inherit a coaction by the motivic Hopf algebra $\mathcal{A}^{\mathcal{M T}}$. To see what this coaction should be requires introducing motivic multiple zetas, for which the independence in different weights (3.7) is automatic.

### 3.2. Motivic multiple zeta values.

In [5], Goncharov showed how to lift the ordinary iterated integrals $I\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)$, where $a_{i} \in \overline{\mathbb{Q}}$ to periods of mixed Tate motives. In the case where the $a_{i} \in\{0,1\}$, he showed that these motives are unramified over $\mathbb{Z}$ (see also [6]), and therefore define objects in $\mathcal{A}^{\mathcal{M} \mathcal{T}}$. In his version of motivic multiple zeta values, the element corresponding to $\zeta(2)$ is zero.

One can show using the formalism of [4] that these can in turn be lifted to elements of $\mathcal{H}^{\mathcal{M}}+$ in such a way that the motivic version of $\zeta(2)$ is non-zero. However, the tollation involves making some choices (see [1], $\S 2$ for the definitions). In summary, there is a graded algebra

$$
\mathcal{H}=\bigoplus_{n \geq 0} \mathcal{H}_{n}
$$

of motivic multiple zeta values with the following properties:

- The vector space underlying $\mathcal{H}_{n}$ is the quotient of the $\mathbb{Q}$ vector space spanned by symbols $\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)$ where
$a_{0}, \ldots, a_{n+1} \in\{0,1\}$, modulo some (non-explicit) relations. The class of such a symbol is denoted

$$
\begin{equation*}
I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right) \in \mathcal{H}_{n} \tag{3.9}
\end{equation*}
$$

and is called a motivic iterated integral. Elements of $\mathcal{H}_{n}$ are said to have weight $n$. Examples of relations between the elements (3.9) are (compare lemma 2.2):

10: $I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)=0$ if $a_{0}=a_{n+1}$ and $n \geq 1$.
I1: $I^{\mathrm{m}}\left(a_{0} ; a_{1} ; a_{2}\right)=0$ for all $a_{0}, a_{1}, a_{2} \in\{0,1\}$, and $I^{\mathrm{m}}\left(a_{0} ; a_{1}\right)=1$ for all $a_{0}, a_{1} \in\{0,1\}$.
I2: $I^{\mathrm{m}}\left(0 ; a_{1}, \ldots, a_{n} ; 1\right)=(-1)^{n} I^{\mathrm{m}}\left(1 ; a_{n}, \ldots, a_{1} ; 0\right)$.
I3: $I^{\mathrm{m}}\left(0 ; a_{1}, \ldots, a_{n} ; 1\right)=(-1)^{n} I^{\mathrm{m}}\left(0 ; 1-a_{n}, \ldots, 1-a_{1} ; 1\right)$.
The algebra structure on $\mathcal{H}$ is given by the shuffle product:

$$
\begin{aligned}
I^{\mathrm{m}}\left(x ; a_{1}, \ldots, a_{r} ; y\right) I^{\mathrm{m}}\left(x ; a_{r+1}, \ldots, a_{r+s} ; y\right)= \\
\quad \sum_{\sigma \in \Sigma(r, s)} I^{\mathrm{m}}\left(x ; a_{\sigma(1)}, \ldots, a_{\sigma(r+s)} ; y\right),
\end{aligned}
$$

for any $a_{i}, x, y \in\{0,1\}$.

- There is a well-defined map (the period)

$$
\begin{align*}
\text { per: } \mathcal{H} & \rightarrow \mathbb{R}  \tag{3.10}\\
I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right) & \longrightarrow I\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)
\end{align*}
$$

which is a ring homomorphism. In particular, all relations satisfied by the $I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)$ are also satisfied by the iterated integrals $I\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)$.

- Let $n_{1}, \ldots, n_{r} \in \mathbb{N}_{+}$, where $n_{r} \geq 2$. Define the motivic multiple zeta value to be

$$
\zeta^{\mathfrak{m}}\left(n_{1}, \ldots, n_{r}\right)=(-1)^{r} I^{\mathfrak{m}}\left(0 ; \rho\left(n_{1}, \ldots, n_{r}\right) ; 1\right)
$$

Its period is $\zeta\left(n_{1}, \ldots, n_{r}\right)$. The element $\zeta^{\mathfrak{m}}(2) \in \mathcal{H}_{2}$ is nonzero, since its period is $\zeta(2) \neq 0$. One easily shows using relations $\mathbf{I 0} \mathbf{- I} \mathbf{I}$ that every generator (3.9) is a linear combination of $\zeta^{\mathfrak{m}}\left(n_{1}, \ldots, n_{r}\right)$, where $n_{i} \geq 1$ and $n_{r} \geq 2$.

- Let $\mathcal{A}=\mathcal{H} / \zeta^{\mathfrak{m}}(2) \mathcal{H}$. It is graded by the weight, so we write $\mathcal{A}=\bigoplus_{n \geq 0} \mathcal{A}_{n}$. Then $\mathcal{A}$ is a Hopf subalgebra of $\mathcal{A}^{\mathcal{M T}}$ and $\mathcal{H}$ is an algebra-comodule over $\mathcal{A}$. Thus there is a coaction

$$
\Delta: \mathcal{H} \longrightarrow \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}
$$

which we describe explicitly in $\S 3.4$. One can show from the formula given in $\S 3.4$ that $\Delta \zeta^{\mathfrak{m}}(2)=1 \otimes \zeta^{\mathfrak{m}}(2)$.

- There is a non-canonical isomorphism $\mathcal{H} \cong \mathcal{A} \otimes_{\mathbb{Q}} \mathbb{Q}\left[\zeta^{\mathfrak{m}}(2)\right]$. Since $\mathcal{A} \hookrightarrow \mathcal{A}^{\mathcal{M} \mathcal{T}}$ it follows that there is a non-canonical embedding of graded algebra-comodules

$$
\begin{equation*}
\mathcal{H} \hookrightarrow \mathcal{H}^{\mathcal{M} \mathcal{T}_{+}} \tag{3.11}
\end{equation*}
$$

which maps $\zeta^{\mathfrak{m}}(2)$ to $f_{2}$.
Remark 3.5. The relations between the motivic multiple zeta values $\zeta^{\mathfrak{m}}\left(n_{1}, \ldots, n_{r}\right)$ are not known explicitly, but a standard conjecture states that they are given by the regularized double shuffle relations (it is not presently known if there are more relations). One does not need to know these relations (in fact, any relations besides those given above) in order to do effective computations with motivic multiple zeta values.

Remark 3.6. The formalism described above is rather powerful. For instance, it immediately implies that

$$
\operatorname{dim}_{\mathbb{Q}} \mathcal{Z}_{k} \stackrel{(3.10)}{\leq} \operatorname{dim}_{\mathbb{Q}} \mathcal{H}_{k} \stackrel{(3.11)}{\leq} \operatorname{dim}_{\mathbb{Q}} \mathcal{H}_{k}^{\mathcal{M} \mathcal{T}_{+}}=d_{k}
$$

where the numbers $d_{k}$ are defined by (3.6). The first inequality arises because per : $\mathcal{H}_{k} \rightarrow \mathcal{Z}_{k}$ is surjective. The bound $\operatorname{dim}_{\mathbb{Q}} \mathcal{Z}_{k} \leq d_{k}$ was first proved independently by Goncharov (see Deligne-Goncharov [4]) and Terasoma [8]. The main result of [1] is the lower bound $\operatorname{dim}_{\mathbb{Q}} \mathcal{H}_{k} \geq d_{k}$, which in turn implies that (3.11) is an isomorphism. We shall not need this fact for the sequel. It is not known if $\operatorname{dim} \mathcal{Z}_{k}>1$ for any $k$.

The various choices made above (namely (3.5) and (3.11)) will be absorbed into a single morphism of graded algebra-comodules

$$
\begin{equation*}
\phi: \mathcal{H} \longrightarrow \mathcal{U} \tag{3.12}
\end{equation*}
$$

which is obtained by composing (3.11) with (3.5). It maps $\zeta^{\mathfrak{m}}(2)$ to $f_{2}$, and induces a morphism of Hopf algebras $\phi: \mathcal{A} \rightarrow \mathcal{U}^{\prime}$ which only depends on (3.5), i.e., a choice of generators of the motivic Lie algebra.

### 3.3. Notations

The motivic multiple zeta values can exist on three different levels: the highest being the comodule $\mathcal{H}$; next the Hopf algebra

$$
\mathcal{A}=\mathcal{H} / \zeta^{\mathfrak{m}}(2) \mathcal{H}
$$

in which $\zeta^{\mathfrak{m}}(2)$ is killed; and finally the Lie coalgebra

$$
\begin{equation*}
\mathcal{L}=\frac{\mathcal{A}_{>0}}{\mathcal{A}_{>0} \mathcal{A}_{>0}}, \tag{3.13}
\end{equation*}
$$

of indecomposable elements of $\mathcal{A}$. We use the notation $\zeta^{\mathfrak{m}}$ to denote an element in $\mathcal{H} ; \zeta^{\mathfrak{a}}$ its image in $\mathcal{A}$; and $\zeta^{\mathfrak{L}}$ its image in $\mathcal{L}$ :

$$
\begin{array}{ccccc}
\mathcal{H}_{>0} & \longrightarrow & \mathcal{A}_{>0} & \longrightarrow & \mathcal{L}  \tag{3.14}\\
\Psi & & \Psi & & \cup \\
\zeta^{\mathfrak{m}}(w) & \mapsto & \zeta^{\mathfrak{a}}(w) & \mapsto & \zeta^{\mathfrak{L}}(w) .
\end{array}
$$

Thus the elements $\zeta^{\mathfrak{a}}\left(n_{1}, \ldots, n_{r}\right)$ are exactly the motivic multiple zeta values considered by Goncharov in [5], and $\zeta^{\mathfrak{a}}(2)=0$. We use the same superscripts for the motivic iterated integrals, viz. $I^{\mathrm{m}}, I^{a}, I^{\mathfrak{L}}$.

### 3.4. Formula for the coaction

Goncharov computed the coproduct $\Delta: \mathcal{A} \rightarrow \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{A}$ on the elements $I^{a}\left(a_{0} ; \ldots ; a_{n+1}\right)$ in [5], Theorem 1.2. The coaction on $\mathcal{H}$ is essentially given by the same formula (see [1], $\S 2$ ).

Theorem 3.7. The coaction

$$
\begin{equation*}
\Delta: \mathcal{H} \longrightarrow \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H} \tag{3.15}
\end{equation*}
$$

can be computed explicitly as follows. For any $a_{0}, \ldots, a_{n+1} \in\{0,1\}$, the image of a generator $\Delta I^{\mathfrak{m}}\left(a_{0} ; a_{1}, \ldots, a_{n} ; a_{n+1}\right)$ is given by

$$
\begin{array}{r}
\sum_{i_{0}<i_{1}<\ldots<i_{k}<i_{k+1}}\left(\prod_{p=0}^{k} I^{a}\left(a_{i_{p}} ; a_{i_{p}+1}, \ldots, a_{i_{p+1}-1} ; a_{i_{p+1}}\right)\right) \otimes  \tag{3.16}\\
I^{\mathrm{m}}\left(a_{0} ; a_{i_{1}}, \ldots, a_{i_{k}} ; a_{n+1}\right)
\end{array}
$$

where the sum is over indices satisfying $i_{0}=0$ and $i_{k+1}=n+1$, and all $0 \leq k \leq n$. Note that the trivial elements $I^{a}(a ; b)$ are equal to 1 .

This formula has an elegant interpretation in terms of cutting off segments of a semicircular polygon, for which we refer to [5] for further details. Note that the formula (3.16) is very inefficient for practical and theoretical computations as it contains a huge amount of redundant information. This is the main reason for introducing the derivation operators in $\S 4.3$ below.

### 3.5. Zeta cogenerators

The following lemma ([5], Theorem 6.4) is an easy consequence of the set up of $\S 3.2$, Theorem 3.7, and the fact that $\zeta(2 n+1) \neq 0$.

Lemma 3.8. For $n \geq 1, \zeta^{\mathfrak{m}}(2 n+1) \in \mathcal{H}$ is non-zero and satisfies

$$
\Delta \zeta^{\mathfrak{m}}(2 n+1)=1 \otimes \zeta^{\mathfrak{m}}(2 n+1)+\zeta^{\mathfrak{a}}(2 n+1) \otimes 1 \in \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H} .
$$

Furthermore, Euler's relation for even zeta values implies that

$$
\zeta^{\mathfrak{m}}(2 n)=b_{n} \zeta^{\mathfrak{m}}(2)^{n}
$$

where $b_{n}=(-1)^{n+1} \frac{1}{2} B_{2 n} \frac{(24)^{n}}{(2 n)!}$, and the $B_{2 n}$ are Bernoulli numbers.
We can therefore normalize our choice of map (3.12) so that

$$
\mathcal{H} \xrightarrow{\phi} \mathcal{U}
$$

maps $\zeta^{\mathfrak{m}}(2 n+1)$ to $f_{2 n+1}$. For notational convenience we define

$$
\begin{equation*}
f_{2 n}=b_{n} f_{2}^{n} \in \mathcal{U}_{2 n} \tag{3.17}
\end{equation*}
$$

where $b_{n}$ is defined in the previous lemma. We can therefore write:

$$
\begin{equation*}
\phi\left(\zeta^{\mathfrak{m}}(N)\right)=f_{N} \quad \text { for all } \quad N \geq 2 \tag{3.18}
\end{equation*}
$$

Remark 3.9. If $\xi \in \mathcal{H}$ is of weight $N$ then $\xi^{\prime}=\xi+\alpha \zeta^{\mathfrak{m}}(N)$, for any $\alpha \in \mathbb{Q}$, cannot be distinguished from $\xi$ using the coaction $\Delta$. This is the basic reason why our decomposition algorithm (§5) is not exact.

## §4. Explicit computations with motivic multiple zeta values

The purpose of this paragraph is to explain how to compute the Galois coaction on motivic multiple zeta values explicitly. Since motivic multiple zetas are a torsor over the motivic Galois group, and since we do not have canonical generators of the motivic Lie algebra, we have to make some choices.

The basic idea is that fixing a map $\phi: \mathcal{H}_{\leq N} \hookrightarrow \mathcal{U}_{\leq N}$ in low weights which is compatible with the grading, shuffle multiplication and the respective coactions fixes a choice of generators of the motivic Lie algebra $\sigma_{2 n+1}$ for $2 n+1 \leq N$, and enables us to compute their action on the motivic multiple zeta values in all weights (in $\S 5$, such a $\phi$ will be determined by a choice of polynomial basis of $\mathcal{H}_{\leq N}$ ). Thus the choice of $\phi$ gives derivation operators for all $1<2 n+1 \leq N$ :

$$
\partial_{2 n+1}^{\phi}: \mathcal{H}_{m} \rightarrow \mathcal{H}_{m-2 n-1} \quad \text { for all } m \geq 2 n+1
$$

which can be computed explicitly from an infinitesimal version of the coaction (3.15), and a certain coefficient function $c_{2 n+1}^{\phi}: \mathcal{H}_{2 n+1} \rightarrow \mathbb{Q}$ which is derived from $\phi$. One advantage is that the infinitesimal coaction (which we denote by operators $D_{2 n+1}$ defined below) enormously simplifies the formula (3.16) for the full coaction.

### 4.1. Derivation operators on the model $\mathcal{U}$

In order to detect elements in $\mathcal{U}$ we can use a set of derivations as follows. For each $n \geq 1$, define linear maps by

$$
\begin{align*}
\partial_{2 n+1}: \mathbb{Q}\left\langle f_{3}, f_{5}, \ldots\right\rangle & \rightarrow \mathbb{Q}\left\langle f_{3}, f_{5}, \ldots\right\rangle  \tag{4.1}\\
\partial_{2 n+1}\left(f_{i_{1}} \ldots f_{i_{r}}\right) & = \begin{cases}f_{i_{2}} \ldots f_{i_{r}}, & \text { if } i_{1}=2 n+1, \\
0, & \text { otherwise }\end{cases}
\end{align*}
$$

It is easy to verify that $\partial_{2 n+1}$ is a derivation for the shuffle product, i.e.,

$$
\partial_{2 n+1}(a \amalg b)=\partial_{2 n+1}(a) \amalg b+a \amalg \partial_{2 n+1}(b),
$$

for any $a, b \in \mathbb{Q}\left\langle f_{3}, f_{5}, \ldots\right\rangle$. The map $\partial_{2 n+1}$ decreases the motivic depth by 1 , and the weight by $2 n+1$. If we set $\partial_{2 n+1}\left(f_{2}\right)=0$, then the maps $\partial_{2 n+1}$ uniquely extend to derivations:

$$
\partial_{2 n+1}: \mathcal{U} \longrightarrow \mathcal{U}
$$

Definition 4.1. Let $\partial_{<N}$ be the sum of $\partial_{2 i+1}$ for $1<2 i+1<N$ :

$$
\begin{equation*}
\partial_{<N}: \mathcal{U}_{N} \longrightarrow \bigoplus_{1 \leq i<\left\lfloor\frac{N}{2}\right\rfloor} \mathcal{U}_{N-2 i-1} \tag{4.2}
\end{equation*}
$$

Lemma 4.2. The following sequence is exact:

$$
\begin{equation*}
0 \longrightarrow f_{N} \mathbb{Q} \longrightarrow \mathcal{U}_{N} \xrightarrow{\partial_{<N}} \bigoplus_{1 \leq i<\left\lfloor\frac{N}{2}\right\rfloor} \mathcal{U}_{N-2 i-1} \longrightarrow 0 \tag{4.3}
\end{equation*}
$$

Proof. It is clear that every element $F \in \mathcal{U}_{N}$ can be uniquely written in the following form:

$$
\begin{equation*}
F=\sum_{1 \leq i<\left\lfloor\frac{N}{2}\right\rfloor} f_{2 i+1} v_{N-2 i-1}+c f_{N} \tag{4.4}
\end{equation*}
$$

where $c \in \mathbb{Q}$ and the $v_{j} \in \mathcal{U}_{j}$, and the product on the right is concatenation. The elements $v_{N-2 i-1}$ are equal to $\partial_{2 i+1} F$ by definition. Every tuple $\left(v_{N-2 i-1}\right)_{1 \leq i<\left\lfloor\frac{N}{2}\right\rfloor}$ arises in this way. Q.E.D.

Thus by repeatedly applying operators $\partial_{2 i+1}$ for $2 i+1<N$, we can detect elements in $\mathcal{U}_{N}$, up to elements in the kernel $f_{N} \mathbb{Q}$. The reason for this kernel is that, in the multiple zeta setting, these elements are the ones which are invisible to the coaction (Remark 3.9), and can only be detected by the (transcendental) period map.

### 4.2. Hopf algebra interpretation

Recalling that $\mathcal{U}^{\prime}=\mathcal{U} / f_{2} \mathcal{U}$, consider the set of indecomposables:

$$
L=\frac{\mathcal{U}_{>0}^{\prime}}{\mathcal{U}_{>0}^{\prime} \mathcal{U}_{>0}^{\prime}}
$$

which is the cofree graded Lie coalgebra on cogenerators $f_{3}, f_{5}, \ldots$ in all odd degrees $\geq 3$. Its (weight) graded dual $L^{\vee}$ is the free Lie algebra on dual generators $f_{3}^{\vee}, f_{5}^{\vee}, \ldots$ in all negative odd degrees $\leq-3$. In each graded weight $N$ there is a perfect pairing $L_{N} \otimes_{\mathbb{Q}} L_{N}^{\vee} \rightarrow \mathbb{Q}$ of finitedimensional vector spaces. Thus every dual generator defines a map $f_{2 n+1}^{\vee}: L \rightarrow \mathbb{Q}$. Let $\pi: \mathcal{U}_{>0}^{\prime} \rightarrow L$ denote the quotient map, and for $1<2 n+1 \leq N$ consider the map

$$
\begin{equation*}
\mathcal{U} \xrightarrow{\Delta^{\prime}} \mathcal{U}_{>0}^{\prime} \otimes_{\mathbb{Q}} \mathcal{U} \xrightarrow{\pi \otimes i d} L \otimes_{\mathbb{Q}} \mathcal{U} \xrightarrow{f_{2 n+1}^{\vee} \otimes i d} \mathcal{U} \tag{4.5}
\end{equation*}
$$

where $\Delta^{\prime}=\Delta-1 \otimes i d$. It follows from the structure of $\mathcal{U}$ that this map is precisely $\partial_{2 n+1}$ (4.1). Note that (4.5), restricted to $\mathcal{U}_{N}$, factors through:

$$
\begin{equation*}
\mathcal{U}_{N} \longrightarrow \mathcal{U}_{2 n+1}^{\prime} \otimes_{\mathbb{Q}} \mathcal{U}_{N-2 n-1} \xrightarrow{\pi \otimes i d} L_{2 n+1} \otimes_{\mathbb{Q}} \mathcal{U}_{N-2 n-1} \tag{4.6}
\end{equation*}
$$

where the first map is the $(2 n+1, N-2 n-1)$-graded part of $\Delta$.

### 4.3. Derivations on $\mathcal{H}$

Consider the infinitesimal version of (3.16).
Definition 4.3. For each odd $r \geq 3$, and all $m \geq 1$, define

$$
D_{r}: \mathcal{H}_{m} \xrightarrow{\Delta_{r, m-r}} \mathcal{A}_{r} \otimes_{\mathbb{Q}} \mathcal{H}_{m-r} \xrightarrow{\pi \otimes i d} \mathcal{L}_{r} \otimes_{\mathbb{Q}} \mathcal{H}_{m-r}
$$

to be the weight $(r, m-r)$-graded part of the coaction, followed by projection onto the Lie coalgebra. It follows from Theorem 3.7 that the action of $D_{r}$ on the element $I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{m} ; a_{m+1}\right)$ is given by:

$$
\begin{align*}
& \sum_{p=0}^{m-r} I^{\mathfrak{L}}\left(a_{p} ; a_{p+1}, \ldots, a_{p+r} ; a_{p+r+1}\right) \otimes  \tag{4.7}\\
& \quad I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{p}, a_{p+r+1}, \ldots, a_{m} ; a_{m+1}\right)
\end{align*}
$$

Note that this formula is closely related to the Connes-Kreimer coproduct formula for a class of linear graphs with two external legs. By analogy, we call the sequence ( $a_{p} ; a_{p+1}, \ldots, a_{p+r} ; a_{p+r+1}$ ) on the left the subsequence and the sequence ( $a_{0} ; a_{1}, \ldots, a_{p}, a_{p+r+1}, \ldots, a_{m} ; a_{m+1}$ ) on the right the quotient sequence of our original sequence $\left(a_{0} ; a_{1}, \ldots, a_{m} ; a_{m+1}\right)$.

Definition 4.4. Let $N \geq 0$, and observe that $\mathcal{H}_{\leq N} \subset \mathcal{H}$ and $\mathcal{U}_{\leq N} \subset$ $\mathcal{U}$ are subcomodules. A trivialisation of $\mathcal{H}$ up to weight $N$ is a map

$$
\begin{equation*}
\phi: \mathcal{H}_{\leq N} \longrightarrow \mathcal{U}_{\leq N} \tag{4.8}
\end{equation*}
$$

which is homogeneous for the weight, linear, injective, respects the coactions, i.e., $\Delta \phi=\phi \Delta$, and the shuffle multiplication laws, i.e., $\phi\left(x_{1} x_{2}\right)=$ $\phi\left(x_{1}\right) \phi\left(x_{2}\right)$ for all $x_{1}, x_{2} \in \mathcal{H}$ such that $\operatorname{deg} x_{1}+\operatorname{deg} x_{2} \leq N$. We say that such a trivialization $\phi$ is normalized if $\phi\left(\zeta^{\mathfrak{m}}(2)\right)=f_{2}$ and

$$
\begin{equation*}
\phi\left(\zeta^{\mathfrak{m}}(2 n+1)\right)=f_{2 n+1} \tag{4.9}
\end{equation*}
$$

for all $1<2 n+1 \leq N$.
Remark 4.5. We know by [1] that $\operatorname{dim} \mathcal{H}_{\leq N}=\operatorname{dim} \mathcal{U}_{\leq N}$ for all $N$, so any trivialisation (4.8) will automatically be an isomorphism.

The map $\phi$ sends every motivic multiple zeta value of weight less than or equal to $N$ to a non-commutative polynomial in the $f_{i}$ 's. Let $\pi: \mathcal{A}_{>0} \rightarrow \mathcal{L}$ denote the quotient map, where $\mathcal{L}$ is the Lie coalgebra of indecomposables (3.13). Given a trivialisation $\phi$, we denote the map $\mathcal{L}_{\leq N} \rightarrow L_{\leq N}$ induced by (4.8) by $\phi$ also.

Definition 4.6. If $\phi$ is a trivialisation of $\mathcal{H}$ up to weight $N$, then define the coefficient map for all $1<2 n+1 \leq N$, to be

$$
c_{2 n+1}^{\phi}=f_{2 n+1}^{\vee} \circ \phi: \mathcal{L}_{2 n+1} \longrightarrow \mathbb{Q}
$$

We sometimes extend the coefficient map to $\mathcal{A}_{2 n+1}\left(\right.$ or $\mathcal{H}_{2 n+1}$ ) via the natural map, and denote it by $c_{2 n+1}^{\phi}$ also. For an element $\xi \in \mathcal{H}_{2 n+1}$, the number $c_{2 n+1}^{\phi}(\xi)$ is simply the coefficient of $f_{2 n+1}$ in the expansion (4.4) of $\phi(\xi)$ as a non-commutative polynomial in the $f$ 's.

Finally, define operators $\partial_{2 n+1}^{\phi}: \mathcal{H} \rightarrow \mathcal{H}$ by

$$
\begin{equation*}
\partial_{2 n+1}^{\phi}=\left(c_{2 n+1}^{\phi} \otimes i d\right) \circ D_{2 n+1} . \tag{4.10}
\end{equation*}
$$

These define derivations on the whole of $\mathcal{H}$. Their restriction to the set of elements of weight at most $N$ satisfies

$$
\left.\phi \circ \partial_{2 n+1}^{\phi}\right|_{\mathcal{H}_{\leq N}}=\left.\partial_{2 n+1} \circ \phi\right|_{\mathcal{H}_{\leq N}}
$$

for all $1<2 n+1 \leq N$. By analogy with $\partial_{<N}$, we define

$$
\begin{equation*}
\partial_{<N}^{\phi}=\bigoplus_{1 \leq i<\left\lfloor\frac{N}{2}\right\rfloor} \partial_{2 i+1}^{\phi} \tag{4.11}
\end{equation*}
$$

### 4.4. The coefficient map in depth 1

Suppose that $\phi$ is a normalized trivialisation of $\mathcal{H}$ up to weight $N$, and let $1<2 n+1 \leq N$. The coefficient $c_{2 n+1}^{\phi} \zeta^{\mathfrak{m}}(2 n+1)$ is 1 . By the shuffle relations for motivic iterated integrals, one can check that

$$
\begin{equation*}
I^{\mathfrak{m}}(0 ; \underbrace{0, \ldots, 0}_{a}, 1, \underbrace{0, \ldots, 0}_{2 n-a} ; 1)=(-1)^{a+1}\binom{2 n}{a} \zeta^{\mathfrak{m}}(2 n+1) . \tag{4.12}
\end{equation*}
$$

Therefore for any such normalized $\phi$ we have

$$
\begin{equation*}
c_{2 n+1}^{\phi}(I^{\mathfrak{L}}(0 ; \underbrace{0, \ldots, 0}_{a}, 1, \underbrace{0, \ldots, 0}_{2 n-a} ; 1))=(-1)^{a+1}\binom{2 n}{a} \tag{4.13}
\end{equation*}
$$

In the later examples, this equation will be used many times.

### 4.5. Extending a trivialisation $\mathcal{H}$

One way to construct a trivialisation of $\mathcal{H}$ is as follows. Suppose that $\phi: \mathcal{H}_{\leq N} \rightarrow \mathcal{U}_{\leq N}$ is a trivialisation up to weight $N$. Then we have differential operators $\partial_{2 n+1}^{\phi}$ on $\mathcal{H}$ for all $1<2 n+1 \leq N$. Suppose that we wish to extend $\phi$ to a trivialisation $\phi^{\prime}: \mathcal{H}_{\leq N+1} \rightarrow \mathcal{U}_{\leq N+1}$ such that $\left.\phi^{\prime}\right|_{\mathcal{H} \leq N}=\phi$. Then for any $\xi \in \mathcal{H}_{N+1}$ we must have

$$
\partial_{2 n+1} \circ \phi^{\prime}(\xi)=\phi \circ \partial_{2 n+1}^{\phi}(\xi)
$$

for all $1 \leq 2 n+1 \leq N$, by the defining properties of a trivialisation. Since by Lemma 4.3 the kernel of $\partial_{<N+1}$ is one dimensional, this determines $\phi^{\prime}(\xi)$ up to a rational multiple of $f_{N+1}$. This rational multiple, call it $c_{\xi}$, must be chosen consistently for all such $\xi$ in such a way that $\phi^{\prime}$ respects the shuffle products.

The decomposition algorithm of $\S 5$ proceeds by fixing a polynomial basis for $\mathcal{H}_{\leq N+1}$, and by choosing values of $c_{\xi}$ when $\xi$ is a generator of this basis. The values of $\phi^{\prime}$ on the monomials in the basis are then deduced by multiplication. Finally, for a general $\xi \in \mathcal{H}_{N+1}$ we can compute its coefficient $c_{\xi}$ by applying the period map, provided that $\operatorname{dim}_{\mathbb{Q}} \mathcal{H}_{N+1}=\operatorname{dim}_{\mathbb{Q}} \mathcal{U}_{N+1}$ (which we know to hold for all $N$ by Remark 4.5). In general, this last step can only be done by numerical approximation since the period map is transcendental.

Examples 4.7. i). Suppose that $\phi: \mathcal{H}_{\leq 3} \rightarrow \mathcal{U}_{\leq 3}$ is a normalized trivialisation. Then since $\mathcal{H}_{3}=\mathbb{Q} \zeta^{\mathfrak{m}}(3)$, the operator $\partial_{3}^{\phi}$ is uniquely defined. Consider $\zeta^{\mathfrak{m}}(2,3)=I^{\mathfrak{m}}(0 ; 10100 ; 1) \in \mathcal{H}_{5}$. We have

$$
\begin{aligned}
D_{3} I^{\mathrm{m}}(0 ; 10100 ; 1)= & I^{\mathfrak{L}}(1 ; 010 ; 0) \otimes I^{\mathrm{m}}(0 ; 10 ; 1) \\
& +I^{\mathfrak{L}}(0 ; 100 ; 1) \otimes I^{\mathrm{m}}(0 ; 10 ; 1)
\end{aligned}
$$

The reflection relation yields $I^{\mathrm{m}}(1 ; 010 ; 0)=-I^{\mathrm{m}}(0 ; 010 ; 1)$ which equals $2 I^{\mathrm{m}}(0 ; 100 ; 1)$ by (4.12), so we conclude that $D_{3} \zeta^{\mathfrak{m}}(2,3)=$ $3 \zeta^{\mathfrak{L}}(3) \otimes \zeta^{\mathfrak{m}}(2)$, and in particular $\partial_{3}^{\phi} \zeta^{\mathfrak{m}}(2,3)=3 \zeta^{\mathfrak{m}}(2)$. Thus any extension $\phi^{\prime}: \mathcal{H}_{\leq 5} \rightarrow \mathcal{U}_{\leq 5}$ must satisfy $\phi^{\prime}\left(\zeta^{\mathfrak{m}}(2,3)\right)=3 f_{3} f_{2}+c f_{5}$ where $c \in \mathbb{Q}$ remains to be determined.
ii). Now let $\phi: \mathcal{H}_{\leq 5} \rightarrow \mathcal{U}_{\leq 5}$ be a normalized trivialisation, so $\partial_{3}^{\phi}$ and $\partial_{5}^{\phi}$ are defined. Consider $\zeta^{\mathfrak{m}}(4,3)=I^{\mathrm{m}}(0 ; 1000100 ; 1) \in \mathcal{H}_{7}$. We have

$$
\begin{aligned}
D_{3} I^{\mathfrak{m}}(0 ; 1000100 ; 1)= & I^{\mathfrak{L}}(0 ; 100 ; 1) \otimes I^{\mathrm{m}}(0 ; 1000 ; 1) \\
= & \zeta^{\mathfrak{L}}(3) \otimes \zeta^{\mathfrak{m}}(4) \\
D_{5} I^{\mathfrak{m}}(0 ; 1000100 ; 1)= & I^{\mathfrak{L}}(1 ; 00010 ; 0) \otimes I^{\mathfrak{m}}(0 ; 10 ; 1) \\
& +I^{\mathfrak{L}}(0 ; 00100 ; 1) \otimes I^{\mathfrak{m}}(0 ; 10 ; 1) \\
= & 10 \zeta^{\mathfrak{L}}(5) \otimes \zeta^{\mathfrak{m}}(2)
\end{aligned}
$$

Thus $\partial_{3}^{\phi} \zeta^{\mathfrak{m}}(4,3)=\zeta^{\mathfrak{m}}(4)$ and $\partial_{5}^{\phi} \zeta^{\mathfrak{m}}(4,3)=10 \zeta^{\mathfrak{m}}(2)$. Thus for any extension $\phi^{\prime}: \mathcal{H}_{\leq 5} \rightarrow \mathcal{U}_{\leq 5}$, we have $\phi^{\prime}\left(\zeta^{\mathfrak{m}}(4,3)\right)=f_{3} f_{4}+10 f_{5} f_{2}+c f_{7}$, where $c \in \mathbb{Q}$ is to be calculated.

These examples can be depicted graphically as follows. The derivations $D_{2 r+1}$ cut off a segment from the marked semi-circles indicated below. Only the segments which give non-zero contributions are indicated.

$I^{\mathrm{m}}(0 ; 10100 ; 1)$

$I^{\mathrm{m}}(0 ; 1000100 ; 1)$

Remark 4.8. These examples perhaps give the wrong impression that modifying the choice of a normalised map $\phi$ only alters the coefficient of $f_{N}$. This is false: in higher weights, increasingly many coefficients (but not all) will depend on the choice of $\phi$. Note also that to compute the image of $\phi$ on an element $\xi \in \mathcal{H}_{N}$ modulo the coefficient of $f_{N}$ only requires knowing $\phi$ on all sub and quotient sequences of $\xi$.

It follows from (4.3) that the operators $D_{2 r+1}$ yield a lot of explicit information about multiple zeta values and their motivic versions.

As a further illustration of this, consider the family of elements

$$
\zeta^{\mathfrak{m}}(1,3, \ldots, 1,3)=I^{\mathfrak{m}}(0 ; 1100 \ldots 1100 ; 1)
$$

It is easy to verify that $D_{2 r+1} \zeta^{\mathfrak{m}}(1,3, \ldots, 1,3)$ vanishes for all $r \geq 1$. When $r$ is odd, this follows from $\mathbf{I O}$, and when $r$ is even this follows from I2 since consecutive terms cancel. Now for any map $\phi: \mathcal{H} \hookrightarrow \mathcal{U}$ as in (3.5), we can define $\partial_{2 n+1}^{\phi}$ by (4.10). Irrespective of the choice of $\phi$, we have $\partial_{2 r+1}^{\phi} \zeta^{\mathfrak{m}}(1,3, \ldots, 1,3)=0$ for all $r \geq 1$. Therefore by (4.3) the element $\zeta^{\mathfrak{m}}(1,3, \ldots, 1,3)$ is a rational multiple of $\zeta^{\mathfrak{m}}(N)$, where $N$ is its weight. On taking the period map we deduce that

$$
\zeta(\underbrace{1,3, \ldots, 1,3}_{n})=\alpha_{n} \pi^{4 n}
$$

for some $\alpha_{n} \in \mathbb{Q}$. David Broadhurst showed that $\alpha_{n}=\frac{1}{(2 n+1)(4 n+1)!}$.

## §5. Decomposition of motivic multiple zetas into a basis

By using the comodule structure of $\mathcal{U}$ and the explicit formula for the operators $D_{2 r+1}$, one obtains an 'exact-numerical' algorithm for the decomposition of multiple zeta values into any predefined polynomial basis, along the lines of $\S 4.5$.

### 5.1. Preliminary definitions

Suppose that we wish to decompose multiple zeta values up to some weight $M \geq 2$. We need the following set-up.
1). For $2 \leq N \leq M$ let $V_{N}$ be the $\mathbb{Q}$-vector space spanned by symbols:

$$
\begin{equation*}
\zeta^{\mathfrak{m}}\left(n_{1}, \ldots, n_{r}\right) \tag{5.1}
\end{equation*}
$$

where $n_{i} \geq 1, n_{r} \geq 2$, and $n_{1}+\ldots+n_{r}=N$. We call $N$ the weight. We also represent these elements another way using a different set of
symbols

$$
\begin{equation*}
I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{N} ; a_{N+1}\right) \quad \text { where } a_{i} \in\{0,1\} \tag{5.2}
\end{equation*}
$$

Any symbol (5.2) can be reduced to a linear combination of elements of the form (5.1) using the following relations:

R0: For $n_{i} \geq 1, n_{r} \geq 2$, and $n_{1}+\ldots+n_{r}=N$, we set

$$
I^{\mathfrak{m}}(0 ; \underbrace{1,0, \ldots, 0}_{n_{1}}, \ldots, \underbrace{1,0, \ldots, 0}_{n_{r}} ; 1)=(-1)^{r} \zeta^{\mathfrak{m}}\left(n_{1}, \ldots, n_{r}\right) \in V_{N}
$$

R1: $I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{N} ; a_{N+1}\right)=0$ if $a_{0}=a_{N+1}$ or $a_{1}=\ldots=$ $a_{N}$.

R2: For $k, n_{1}, \ldots, n_{r} \geq 1$,

$$
\begin{gathered}
(-1)^{k} I^{\mathrm{m}}(0 ; \underbrace{0, \ldots, 0}_{k}, \underbrace{1,0, \ldots, 0}_{n_{1}}, \ldots, \underbrace{1,0, \ldots, 0}_{n_{r}} ; 1)= \\
\sum_{i_{1}+\ldots+i_{r}=k}\binom{n_{1}+i_{1}-1}{i_{1}} \ldots\binom{n_{r}+i_{r}-1}{i_{r}} I^{\mathrm{m}}(0 ; \underbrace{1,0, \ldots, 0}_{n_{1}+i_{1}}, \ldots, \underbrace{1,0, \ldots, 0}_{n_{r}+i_{r}} ; 1) .
\end{gathered}
$$

R3: $I^{\mathrm{m}}\left(0 ; a_{1}, \ldots, a_{N} ; 1\right)=(-1)^{N} I^{\mathrm{m}}\left(1 ; a_{N}, \ldots, a_{1} ; 0\right)$.
R4: $I^{\mathrm{m}}\left(0 ; a_{1}, \ldots, a_{N} ; 1\right)=(-1)^{N} I^{\mathrm{m}}\left(0 ; 1-a_{N}, \ldots, 1-a_{1} ; 1\right)$.
To see this, take any element of the form (5.2) and use R1 and R3 to ensure that $a_{0}=0$ and $a_{N+1}=1$. Then use $\mathbf{R 2}$ to rewrite it as a linear combination of elements satisfying $a_{1}=1$. By R4 this ensures that $a_{N}=0$ and finally apply $\mathbf{R 2}$ once more to force $a_{1}=1$. Conclude using R0.

Remark 5.1. Relations R0 and R4 actually induce an extra relation (known as duality) on the generators (5.1). One could take the quotient of $V_{N}$ modulo this relation if one chooses, but we shall not do this here.

Finally, for any generator of $V_{N}$, define its period to be the real number

$$
\begin{equation*}
\operatorname{per}\left(\zeta^{\mathfrak{m}}\left(n_{1}, \ldots, n_{r}\right)\right)=\zeta\left(n_{1}, \ldots, n_{r}\right) \in \mathbb{R} \tag{5.3}
\end{equation*}
$$

2). For $2 \leq N \leq M$ define a $\mathbb{Q}$-vector space $\mathcal{U}_{N}$ with basis elements

$$
\begin{equation*}
f_{2 i_{1}+1} \ldots f_{2 i_{r}+1} f_{2}^{k} \tag{5.4}
\end{equation*}
$$

where $r, k \geq 0, i_{1}, \ldots, i_{r} \geq 1$, and $2\left(i_{1}+\ldots+i_{r}\right)+r+2 k=N$. We also need the multiplication rule $\mathrm{m}: \mathcal{U}_{m} \times \mathcal{U}_{n} \rightarrow \mathcal{U}_{m+n}$ defined by

$$
\begin{array}{r}
f_{2 i_{1}+1} \ldots f_{2 i_{r}+1} f_{2}^{k} \amalg f_{2 i_{r+1}+1} \ldots f_{2 i_{r+s}+1} f_{2}^{\ell} \\
=\sum_{\sigma \in \Sigma(r, s)} f_{2 i_{\sigma(1)}+1} \ldots f_{2 i_{\sigma(r+s)}+1} f_{2}^{k+\ell}
\end{array}
$$

where $\Sigma(r, s)$ is the set of $(r, s)$ shuffles, i.e., permutations $\sigma$ of $1, \ldots, r+s$ such that $\sigma^{-1}(1)<\ldots<\sigma^{-1}(r)$ and $\sigma^{-1}(r+1)<\ldots<\sigma^{-1}(r+s)$.
3). Suppose that we have some conjectural polynomial basis of (motivic) multiple zeta values $B \subset \bigoplus_{2 \leq n \leq M} V_{n}$ up to weight $M$. We shall assume that $B$ contains the elements

$$
B^{0}=\left\{\zeta^{\mathfrak{m}}(2)\right\} \cup\left\{\zeta^{\mathfrak{m}}(3), \zeta^{\mathfrak{m}}(5), \ldots, \zeta^{\mathfrak{m}}(2 r+1)\right\}
$$

where $r$ is the largest integer such that $2 r+1 \leq M$. Denote the remaining elements of $B$ by $B^{\prime}=B \backslash B^{0}$, and let $B_{n}$ denote the set of elements of $B$ of weight $n$. For $2 \leq N \leq M$, let $\langle B\rangle_{N}$ denote the $\mathbb{Q}$-vector space spanned by monomials in elements of the set $B$ which are of total weight $N$, where the weight is additive with respect to multiplication. Part of the decomposition algorithm is to verify that $B$ is indeed a polynomial basis for the (motivic) multiple zeta values. As a first check, one should have

$$
\begin{equation*}
\operatorname{dim}_{\mathbb{Q}}\langle B\rangle_{N}=d_{N} \text { for all } 2 \leq N \leq M, \tag{5.5}
\end{equation*}
$$

where $d_{0}=1, d_{1}=0, d_{2}=1$ and $d_{k}=d_{k-2}+d_{k-3}$ for $k \geq 3$. The integer $d_{N}$ is the dimension of the vector space $\mathcal{U}_{N}$.

### 5.2. Inductive definition of the algorithm

The algorithm is defined by induction on the weight and has two parts:
(1) For all $n \leq N$, we construct a map

$$
\phi: B_{n} \rightarrow \mathcal{U}_{n},
$$

which assigns a $\mathbb{Q}$-linear combination of monomials of the form (5.4) to every element of our basis $B$ of weight at most $N$. Using the multiplication law $m$, extend this map multiplicatively to monomials in the elements of $B$ to give a map

$$
\rho:\langle B\rangle_{n} \longrightarrow \mathcal{U}_{n}
$$

for all $n \leq N$. We require that $\rho$ be an isomorphism to continue (otherwise, the present choice $B$ is not a polynomial basis).
(2) An algorithm to extend $\phi$ to the whole of $V_{n}$ :

$$
\begin{equation*}
\phi: V_{n} \longrightarrow \mathcal{U}_{n} \tag{5.6}
\end{equation*}
$$

for all $n \leq N$. Thus there is an algorithm to assign a $\mathbb{Q}$-linear combination of monomials of the form (5.4) to every element (5.1), but note that it does not actually need to be computed explicitly on all elements of $V_{n}$, only on the basis elements $B_{n}$.
Once (1) and (2) have been constructed, they give a way to decompose any element $\xi \in V_{N}$ as a polynomial in our basis: simply compute

$$
\rho^{-1}(\phi(\xi)) \in\langle B\rangle_{N}
$$

Computing $\rho^{-1}$ involves inverting a square matrix which is of size $d_{N}$, where $d_{N}$ is defined by (3.6) (one could do better by exploiting the motivic depth filtration if one wished).

We now show how to define (1) and (2) by a bootstrapping procedure. Suppose that they have been constructed up to and including weight $N$. For the initial case $N=2$, simply set $\phi\left(\zeta^{\mathfrak{m}}(2)\right)=f_{2}$.

From (2), we have an algorithm to compute a set of coefficient functions

$$
\begin{equation*}
c_{2 r+1}^{\phi}: V_{2 r+1} \longrightarrow \mathbb{Q} \tag{5.7}
\end{equation*}
$$

for all $2 r+1 \leq N$, which to any element $\xi \in V_{2 r+1}$ takes the coefficient of the monomial $f_{2 r+1}$ in $\phi(\xi) \in \mathcal{U}_{2 r+1}$. The induction steps are:

Step 1. Define $\phi$ on elements $\xi \in B_{N+1}$ as follows. If $\xi=\zeta^{\mathfrak{m}}(2 n+1)$ then set $\phi(\xi)=f_{2 n+1}$. Otherwise, write $\xi$ (or $-\xi$ ) in the form

$$
\begin{equation*}
\xi=I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{N+1} ; a_{N+2}\right) \tag{5.8}
\end{equation*}
$$

where $a_{i} \in\{0,1\}$, using relation R0. Define for all $3 \leq 2 r+1 \leq N$,

$$
\begin{align*}
\xi_{2 r+1}= & \sum_{p=0}^{N+1-2 r} c_{2 r+1}^{\phi}\left(I^{\mathrm{m}}\left(a_{p} ; a_{p+1}, \ldots, a_{p+2 r+1} ; a_{p+2 r+2}\right)\right) \times  \tag{5.9}\\
& \phi\left(I^{\mathrm{m}}\left(a_{0} ; a_{1}, \ldots, a_{p}, a_{p+2 r+2}, \ldots, a_{N+1} ; a_{N+2}\right)\right)
\end{align*}
$$

Then $\xi_{2 r+1} \in \mathcal{U}_{N-2 r}$. The right hand side of the product is computed using the algorithm for $\phi$ in strictly lower weights (5.6). Finally, define

$$
\phi(\xi)=\sum_{3 \leq 2 r+1 \leq N} f_{2 r+1} \xi_{2 r+1}
$$

where the product on the right is concatenation. Having computed $\phi$ explicitly on the elements of $B_{N+1}$, compute the map $\rho:\langle B\rangle_{N+1} \rightarrow$ $\mathcal{U}_{N+1}$ by extending $\phi$ by multiplicativity with respect to II , and check that it is an isomorphism. If not, then the choice of $B$ is not a basis. In the case when the basis $B$ contains linear combinations of terms of the form (5.8), $\phi$ is computed in exactly the same way by linearity.

Step 2. The algorithm to compute $\phi$ on any generator $\xi \in V_{N+1}$ proceeds as follows. As above, write $\xi$ in the form (5.8), and compute $\xi_{2 r+1}$ for $3 \leq 2 r+1 \leq N$ using the formula (5.9). As before, let

$$
u=\sum_{3 \leq 2 r+1 \leq N} f_{2 r+1} \xi_{2 r+1}
$$

Then $u$ is an element of $\mathcal{U}_{N+1}$, and we can compute $\rho^{-1}(u) \in\langle B\rangle_{N+1}$ as a polynomial in our basis $B$. The general theory tells us that

$$
\begin{equation*}
c_{\xi}=\frac{\operatorname{per}\left(\xi-\rho^{-1}(u)\right)}{\zeta(N+1)} \in \mathbb{R} \tag{5.10}
\end{equation*}
$$

is a rational number. Compute it to as many digits as required in order to identify this rational to a satisfactory degree of certainty. Define

$$
\phi(\xi)=u+c_{\xi} f_{N+1}
$$

where $f_{2 n}=\frac{\zeta(2 n)}{\zeta(2)^{n}} f_{2}^{n}$ in the case where $N+1=2 n$ is even.
Some worked examples of this algorithm are computed in $\S 6$.

### 5.3. Comments

i). In order to decompose an element $\zeta^{\mathfrak{m}}\left(n_{1}, \ldots, n_{r}\right)$ of weight $N$ into the basis, one must also decompose all the sub and quotient sequences of $I^{\mathrm{m}}\left(0 ; \rho\left(n_{1}, \ldots, n_{r}\right) ; 1\right)$ as they occur in the definition of $D_{2 r+1}$. Since such sequences have strictly smaller weight (the weight decreases by at least 3 ) and strictly smaller depth (numbers of 1 's), the total number of decompositions is manageable.
ii). The computation of the coefficients (5.10) requires an efficient numerical method for computing the multiple zeta values. There are many ways to do this. A simplistic way is to write the path from 0 to 1 as the composition of paths from 0 to $\frac{1}{2}$ and then from $\frac{1}{2}$ to 1 , and use the composition of paths formula. The upshot is that every multiple zeta value can be written in terms of multiple polylogarithms evaluated at $\frac{1}{2}$. Many other methods are also available.
iii). This is only an algorithm in the true sense of the word in so far as it is possible to compute the coefficients $c_{\xi}(5.10)$, and this is the only transcendental input. A different realization of the motivic multiple zeta values (say, in the $p$-adic or even finite mod $p$ setting) might lead to an exact algorithm for the computation of these coefficients too. We hope that one can give a theoretical upper bound for the prime powers which can occur in the denominators $c_{\xi}$ as a function of the weight (and choice of basis).
iv). There is in fact no reason to suppose that our basis contains the depth one elements $\zeta^{\mathfrak{m}}(2 n+1)$. For example, in [1] we proved that the set of Lyndon words ${ }^{1}$ in the Hoffman elements:

$$
\begin{equation*}
\zeta^{\mathfrak{m}}\left(n_{1}, \ldots, n_{r}\right), \text { where } n_{i} \in 2,3 \tag{5.11}
\end{equation*}
$$

is a polynomial basis for $\mathcal{H}$, as conjectured in [2]. This choice of basis gives a canonical trivialisation $\phi: \mathcal{H} \xrightarrow{\sim} \mathcal{U}$ which respects the coactions and satisfies

$$
\begin{aligned}
& c_{2 n+1}^{\phi} \zeta^{\mathfrak{m}}(3, \underbrace{2, \ldots, 2}_{n-1})=(-1)^{n} 2 n\left(2 n-3+2^{1-2 n}\right) \\
& c_{2 n+1}^{\phi} \zeta^{\mathfrak{m}}\left(n_{1}, \ldots, n_{r}\right)=0 \text { if at least two } n_{i} \text { 's are equal to } 3,
\end{aligned}
$$

where $\left(n_{1}, \ldots, n_{r}\right)$ is a Lyndon word in $\{2,3\}$. The equation for the coefficient of $\zeta^{\mathfrak{m}}(3,2, \ldots, 2)$ follows from a theorem of Zagier's [9]. The previous algorithm allows one to decompose MZV's into this basis too.
$v)$. A similar version of this algorithm also works for multiple polylogarithms evaluated at $N^{\text {th }}$ roots of unity, in particular in the case of Euler sums $(N=2)$. In some cases an explicit basis for the motivic iterated integrals at roots of unity is known by [3]. In the case $N=2$, this basis was conjectured by Broadhurst.
vi). Given a relation between motivic multiple zeta values, one can define operators $\partial_{2 n+1}^{\phi}$ (for some choice of $\phi$ ), to obtain more relations of lower weight. Applying the period map gives a relation between real MZV's. Thus a relation between motivic MZV's gives rise to a family of relations between real MZV's.

The converse is also true: the decomposition algorithm allows one to prove an identity between motivic MZV's if one knows sufficiently many relations between real MZV's to determine all the coefficients (5.10)

[^1]which arise in the algorithm. This was alluded to in point (2) of the introduction. In ([1], §4) this idea was used to lift an identity between real MZV's to the motivic level (it is essentially the definition of the motivic MZV's).

## §6. Worked example of the decomposition algorithm

We use the following set of motivic multiple zeta values as our independent algebra generators up to weight 10 (compare the tables in §2.5):

$$
\begin{equation*}
B=\left\{\zeta^{\mathfrak{m}}(2), \zeta^{\mathfrak{m}}(3), \zeta^{\mathfrak{m}}(5), \zeta^{\mathfrak{m}}(7), \zeta^{\mathfrak{m}}(3,5), \zeta^{\mathfrak{m}}(9), \zeta^{\mathfrak{m}}(3,7)\right\} \tag{6.1}
\end{equation*}
$$

We first associate to each element of $B$ an element in $\mathcal{U}$. To economize on notations, we denote $\partial^{\phi_{B}}$ by $\partial$, since there is no confusion.

### 6.1. Construction of the basis polynomials

The elements $\phi^{B}(b) \in \mathcal{U}$, for $b \in B$, are defined as follows. Firstly,

$$
\phi^{B}\left(\zeta^{\mathfrak{m}}(n)\right)=f_{n}, \text { for } n=2,3,5,7,9
$$

by (2) of $\S 5$. By direct application of definition 4.3 we have:

$$
\begin{aligned}
D_{3} \zeta^{\mathfrak{m}}(3,5)= & I^{\mathfrak{L}}(0 ; 100 ; 1) \otimes I^{\mathrm{m}}(0 ; 10000 ; 1) \\
& +I^{\mathfrak{L}}(1 ; 001 ; 0) \otimes I^{\mathrm{m}}(0 ; 10000 ; 1) \\
D_{5} \zeta^{\mathfrak{m}}(3,5)= & I^{\mathfrak{L}}(1 ; 00100 ; 0) \otimes I^{\mathrm{m}}(0 ; 100 ; 1) \\
& +I^{\mathfrak{L}}(0 ; 10000 ; 1) \otimes I^{\mathrm{m}}(0 ; 100 ; 1)
\end{aligned}
$$

By (4.12), $\partial_{3} \zeta^{\mathfrak{m}}(3,5)=0, \partial_{5} \zeta^{\mathfrak{m}}(3,5)=-5 \zeta^{\mathfrak{m}}(3)$, and therefore

$$
\begin{equation*}
\phi^{B}\left(\zeta^{\mathfrak{m}}(3,5)\right)=-5 f_{5} f_{3} \tag{6.2}
\end{equation*}
$$

following the prescription of (2), $\S 5$. Similarly,

$$
\begin{aligned}
D_{3} \zeta^{\mathfrak{m}}(3,7)= & I^{\mathfrak{L}}(0 ; 100 ; 1) \otimes I^{\mathrm{m}}(0 ; 1000000 ; 1) \\
& +I^{\mathfrak{L}}(1 ; 001 ; 0) \otimes I^{\mathfrak{m}}(0 ; 1000000 ; 1) \\
D_{5} \zeta^{\mathfrak{m}}(3,7)= & I^{\mathfrak{L}}(1 ; 00100 ; 0) \otimes I^{\mathrm{m}}(0 ; 10000 ; 1) \\
D_{7} \zeta^{\mathfrak{m}}(3,7)= & I^{\mathfrak{L}}(1 ; 0010000 ; 0) \otimes I^{\mathrm{m}}(0 ; 100 ; 1) \\
& +I^{\mathfrak{L}}(0 ; 1000000 ; 1) \otimes I^{\mathrm{m}}(0 ; 100 ; 1)
\end{aligned}
$$

Thus $\partial_{3} \zeta^{\mathfrak{m}}(3,7)=0, \partial_{5} \zeta^{\mathfrak{m}}(3,7)=-6 \zeta^{\mathfrak{m}}(5), \partial_{7} \zeta^{\mathfrak{m}}(3,7)=-14 \zeta^{\mathfrak{m}}(3)$, i.e.,

$$
\begin{equation*}
\phi^{B}\left(\zeta^{\mathfrak{m}}(3,7)\right)=-14 f_{7} f_{3}-6 f_{5} f_{5} \tag{6.3}
\end{equation*}
$$

This computation proves that $B$ is indeed an algebra basis, since the elements in $\phi^{B}\left(\langle B\rangle_{n}\right)$ for $n \leq 10$ are linearly independent. For example, in weight 10 one checks that we have the following basis for $\mathcal{U}_{10}$ :
$f_{2}^{5}, f_{3} \amalg f_{3} f_{2}^{2}, f_{3} \amalg f_{5} f_{2}, f_{5} \amalg f_{5},-5 f_{5} f_{3} f_{2}, f_{3} \amalg f_{7},-14 f_{7} f_{3}-6 f_{5} f_{5}$.
Therefore any motivic MZV of weight 10 can be uniquely written
$\xi=a_{0} \zeta^{\mathfrak{m}}(2)^{5}+a_{1} \zeta^{\mathfrak{m}}(2)^{2} \zeta^{\mathfrak{m}}(3)^{2}+a_{2} \zeta^{\mathfrak{m}}(2) \zeta^{\mathfrak{m}}(3) \zeta^{\mathfrak{m}}(5)+a_{3} \zeta^{\mathfrak{m}}(5)^{2}$

$$
\begin{equation*}
+a_{4} \zeta^{\mathfrak{m}}(2) \zeta^{\mathfrak{m}}(3,5)+a_{5} \zeta^{\mathfrak{m}}(3) \zeta^{\mathfrak{m}}(7)+a_{6} \zeta^{\mathfrak{m}}(3,7) \tag{6.4}
\end{equation*}
$$

where $a_{0}, \ldots, a_{6} \in \mathbb{Q}$. From the action of $\partial_{3}, \partial_{5}, \partial_{7}$ computed in (6.2), (6.3), we see that the $a_{i}$ are given by applying the following operators

$$
\begin{gather*}
a_{1}=\frac{1}{2} c_{2}^{2} \partial_{3}^{2}, a_{2}=c_{2} \partial_{5} \partial_{3}, a_{3}=\frac{1}{2} \partial_{5}^{2}+\frac{3}{14}\left[\partial_{7}, \partial_{3}\right]  \tag{6.5}\\
a_{4}=\frac{1}{5} c_{2}\left[\partial_{5}, \partial_{3}\right], a_{5}=\partial_{7} \partial_{3}, a_{6}=\frac{1}{14}\left[\partial_{7}, \partial_{3}\right]
\end{gather*}
$$

to the element $\phi^{B}(\xi)$, where $c_{2}^{n}$ means taking the coefficient of $f_{2}^{n}$.

### 6.2. Sample decompositions

Let us compute $\zeta^{\mathfrak{m}}(4,3,3)$ as a polynomial in our basis $B$. From the calculations (4) below, we shall see that its non-trivial sub and quotient sequences are $\zeta^{\mathfrak{m}}(3,4), \zeta^{\mathfrak{m}}(4,3), \zeta^{\mathfrak{m}}(2,3)$. Working backwards, we decompose these elements in increasing order of weight.
(1) Decomposition of $\zeta^{\mathfrak{m}}(2,3)$. By example 4.7, $\partial_{3} \zeta^{\mathfrak{m}}(2,3)=$ $3 \zeta^{\mathfrak{m}}(2)$. In weight five, $\mathcal{U}_{5} \cong \mathbb{Q} f_{3} f_{2} \oplus \mathbb{Q} f_{5}$, so it follows that $\zeta^{\mathfrak{m}}(2,3)$ is of the form $c \zeta^{\mathfrak{m}}(5)+3 \zeta^{\mathfrak{m}}(3) \zeta^{\mathfrak{m}}(2)$, where $c \in \mathbb{Q}$. By numerical computation, or some other method, we check that:

$$
c=\frac{\zeta(2,3)-3 \zeta(2) \zeta(3)}{\zeta(5)} \sim-\frac{11}{2} .
$$

Thus $\zeta^{\mathfrak{m}}(2,3)=-\frac{11}{2} \zeta^{\mathfrak{m}}(5)+3 \zeta^{\mathfrak{m}}(3) \zeta^{\mathfrak{m}}(2)$.
(2) Decomposition of $\zeta^{\mathfrak{m}}(4,3)$. By example 4.7, we have $\partial_{3} \zeta^{\mathfrak{m}}(4,3)$ $=\zeta^{\mathfrak{m}}(4)=\frac{2}{5} \zeta^{\mathfrak{m}}(2)^{2}$, and $\partial_{5} \zeta^{\mathfrak{m}}(4,3)=10 \zeta^{\mathfrak{m}}(2)$. In weight 7,

$$
\mathcal{U}_{7} \cong \mathbb{Q} f_{3} f_{2}^{2} \oplus \mathbb{Q} f_{5} f_{2} \oplus \mathbb{Q} f_{7}
$$

so $\phi^{B}\left(\zeta^{\mathfrak{m}}(4,3)\right)$ is of the form $c f_{7}+10 f_{5} f_{2}+\frac{2}{5} f_{3} f_{2}^{2}$. By numerical computation or otherwise,

$$
c=\frac{\zeta(4,3)-10 \zeta(2) \zeta(5)-\frac{2}{5} \zeta(3) \zeta(2)^{2}}{\zeta(7)} \sim-18
$$

Thus $\zeta^{\mathfrak{m}}(4,3)=-18 \zeta^{\mathfrak{m}}(7)+10 \zeta^{\mathfrak{m}}(5) \zeta^{\mathfrak{m}}(2)+\frac{2}{5} \zeta^{\mathfrak{m}}(3) \zeta^{\mathfrak{m}}(2)^{2}$.
(3) Decomposition of $\zeta^{\mathfrak{m}}(3,4)$. We omit the computation, which is similar, and merely state that $\zeta^{\mathfrak{m}}(3,4)=17 \zeta^{\mathfrak{m}}(7)-$ $10 \zeta^{\mathfrak{m}}(5) \zeta^{\mathfrak{m}}(2)$. (It also follows immediately from (2) and the socalled stuffle relation $\left.\zeta^{\mathfrak{m}}(3) \zeta^{\mathfrak{m}}(4)=\zeta^{\mathfrak{m}}(3,4)+\zeta^{\mathfrak{m}}(4,3)+\zeta^{\mathfrak{m}}(7).\right)$
(4) Decomposition of $\zeta^{\mathfrak{m}}(4,3,3)$. By (4.7) and relations $\mathbf{I 0}-\mathbf{I 2}$,

$$
\begin{aligned}
D_{3} \zeta^{\mathfrak{m}}(4,3,3)= & \left(I^{\mathfrak{L}}(0 ; 100 ; 1)+I^{\mathfrak{L}}(1 ; 001 ; 0)+I^{\mathfrak{L}}(0 ; 100 ; 1)\right) \\
& \otimes I^{\mathfrak{m}}(0 ; 1000100 ; 1) \\
= & \zeta^{\mathfrak{L}}(3) \otimes \zeta^{\mathfrak{m}}(4,3) \\
D_{5} \zeta^{\mathfrak{m}}(4,3,3)= & I^{\mathfrak{L}}(1 ; 00010 ; 0) \otimes I^{\mathfrak{m}}(0 ; 10100 ; 1) \\
& +I^{\mathfrak{L}}(0 ; 00100 ; 1) \otimes I^{\mathfrak{m}}(0 ; 10100 ; 1) \\
= & 10 \zeta^{\mathfrak{L}}(5) \otimes \zeta^{\mathfrak{m}}(2,3)
\end{aligned}
$$

$$
\begin{aligned}
& D_{7} \zeta^{\mathfrak{m}}(4,3,3) \\
& =\left(I^{\mathfrak{L}}(1 ; 1000100 ; 0)+I^{\mathfrak{L}}(1 ; 0001001 ; 0)+I^{\mathfrak{L}}(0 ; 0100100 ; 1)\right) \\
& \quad \otimes I^{\mathfrak{m}}(0 ; 100 ; 1) \\
& =\left(\zeta^{\mathfrak{L}}(4,3)-\zeta^{\mathfrak{L}}(3,4)-3\left(\zeta^{\mathfrak{L}}(4,3)+\zeta^{\mathfrak{L}}(3,4)\right) \otimes \zeta^{\mathfrak{m}}(3)\right.
\end{aligned}
$$

By $(2)$ and $(3), c_{7}^{\phi_{B}}\left(\zeta^{\mathfrak{L}}(4,3)\right)=-18$ and $c_{7}^{\phi_{B}}\left(\zeta^{\mathfrak{L}}(3,4)\right)=17$, and so $\partial_{7} \zeta^{\mathfrak{m}}(4,3,3)=-32 \zeta(3)$. Thus we have:

$$
\begin{aligned}
\phi^{B}\left(\partial_{3} \zeta^{\mathfrak{m}}(4,3,3)\right) & =\phi^{B}\left(\zeta^{\mathfrak{m}}(4,3)\right) \\
& =-18 f_{7}+10 f_{5} f_{2}+\frac{2}{5} f_{3} f_{2}^{2} \\
\phi^{B}\left(\partial_{5} \zeta^{\mathfrak{m}}(4,3,3)\right) & =10 \phi^{B}\left(\zeta^{\mathfrak{m}}(2,3)\right) \\
& =-55 f_{5}+30 f_{3} f_{2} \\
\phi^{B}\left(\partial_{7} \zeta^{\mathfrak{m}}(4,3,3)\right) & =-32 \phi^{B}\left(\zeta^{\mathfrak{m}}(3)\right) \\
& =-32 f_{3}
\end{aligned}
$$

Using the equations (6.5) we conclude that

$$
\begin{aligned}
\zeta^{\mathfrak{m}}(4,3,3)= & a_{0} \zeta^{\mathfrak{m}}(2)^{5}+\frac{1}{5} \zeta^{\mathfrak{m}}(2)^{2} \zeta^{\mathfrak{m}}(3)^{2}+10 \zeta^{\mathfrak{m}}(2) \zeta^{\mathfrak{m}}(3) \zeta^{\mathfrak{m}}(5) \\
& -\frac{49}{2} \zeta^{\mathfrak{m}}(5)^{2}-18 \zeta^{\mathfrak{m}}(3) \zeta^{\mathfrak{m}}(7)-4 \zeta^{\mathfrak{m}}(2) \zeta^{\mathfrak{m}}(3,5)+\zeta^{\mathfrak{m}}(3,7)
\end{aligned}
$$

Finally, by numerical computation, one checks once again that

$$
\zeta(4,3,3)-\left[\frac{1}{5} \zeta(2)^{2} \zeta(3)^{2}+\ldots+\zeta(3,7)\right] \sim \frac{271}{10} \zeta(10)=\frac{4336}{1925} \zeta(2)^{5}
$$

which gives the coefficient $a_{0}$ of $\zeta^{\mathfrak{m}}(2)^{5}$.
In this example the coefficients $a_{1}, a_{2}, a_{4}$ of (6.4) are computed exactly; the others are obtained indirectly via the period map and numerical approximation.

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[^1]:    ${ }^{1} \mathrm{~A}$ sequence $\left(n_{1}, \ldots, n_{r}\right)$ with $n_{i}=2,3$ is a Lyndon word if $\left(n_{1}, \ldots, n_{r}\right)<$ $\left(n_{i}, \ldots, n_{r}\right)$ for all $i \geq 2$ in the lexicographic ordering determined by $3<2$.

