Zinbiel Algebras and Multiple Zeta Values

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Abstract. We build, using the notion of zinbiel algebra, some commutative sub-algebras $C_{u,v}$ inside an algebra of formal iterated integrals. There is a quotient map from this algebra of formal iterated integrals to the algebra of motivic multiple zeta values. Restricting this quotient map to the sub-algebras $C_{u,v}$ gives a morphism of graded commutative algebras with the same graded dimension. This is conjectured to be generically an isomorphism. When $u+v=0$, the image is instead a sub-algebra of the algebra of motivic multiple zeta values.

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1 Introduction

Multiple zeta values are the convergent iterated integrals from 0 to 1 of the differential forms $\omega_0 = dt/t$ and $\omega_1 = dt/(1-t)$. They span an algebra over $\mathbb{Q}$, which has many interesting connections with different domains, including knot theory and perturbative quantum field theory [21, 11]. This algebra is expected to be graded by the weight, and a famous conjecture of Zagier [22] states that the dimensions of homogeneous components are given by the Padovan numbers. The algebra $\mathsf{A}_{\mathsf{MZV}}$ of motivic multiple zeta values is a more subtle construction, in the setting of periods and mixed motives [5, 6, 11]. It can be defined as the quotient of the commutative algebra $\mathsf{A}_{1,0}$, whose elements are seen as formal iterated integrals of ω_0 and ω_1 from 0 to 1, by the non-explicit ideal of all relations that can be proved using algebraic geometry. This algebra is known to be graded by the weight and its dimensions are given by the Padovan sequence, by results of Brown [5].

There is a surjective morphism, called the period map, from the motivic algebra $\mathsf{A}_{\mathsf{MZV}}$ to the usual algebra of multiple zeta values, defined by taking the numerical value of a formal iterated integral. This period map is expected to be injective, hence an isomorphism.

The aim of this article is to propose an algebraic construction, using the algebraic structures known as zinbiel algebras or dual Leibniz algebras, of some commutative sub-algebras $C_{u,v}$ of $\mathsf{A}_{1,0}$, depending on the choice of two rational numbers u and v.

The notion of zinbiel algebras was introduced under this name around 1995 by Loday in relationship with Leibniz algebras [14]. Their name is the reversal of Leibniz, a play of words justified by the Koszul duality of the two corresponding operads. They have in fact appeared much earlier in 1958 in an article of Schũtzenberger [20, §IV]. Maybe a better name would be "half-shuffle algebras", as they are very closely related to shuffle algebras on words.

The algebras $C_{u,v}$, depending algebraically on the parameters u, v, have the same graded dimensions as the motivic algebra $\mathsf{A}_{\mathsf{MZV}}$. Our main conjecture is then that the restricted quotient map from $C_{u,v}$ to the motivic algebra $\mathsf{A}_{\mathsf{MZV}}$ is generically an isomorphism. In this statement, genericity can be given two distinct meanings: the map is invertible either over the field $\mathbb{Q}(u, v)$ or for an open set of choices of (u, v) in $\mathbb{Q}^2$. In the special case when $u + v = 0$, the image of $C_{u,-u}$ is instead an interesting strict sub-algebra of $\mathsf{A}_{\mathsf{MZV}}$.

One interest of this construction is that it would provide new bases of the algebra $\mathsf{A}_{\mathsf{MZV}}$ indexed by words in 2 and 3. One known basis of $\mathsf{A}_{\mathsf{MZV}}$ is the Hoffman basis [5, 12], given by iterated integrals with at most two consecutive ω_0 and therefore also indexed by words in 2 and 3. Unlike the Hoffman basis, the shuffle product in any of the new candidate bases can be expressed easily in the same basis, as the shuffle product of words. On the negative side, the description of the motivic coaction in these bases is not clear, and the reduction of standard multiple zeta values as a linear combination of the basis is not simple either.

The motivic coaction on the algebra $\mathsf{A}_{\mathsf{MZV}}$ is a very important structure, playing a key rôle in our current understanding of this algebra. If $C_{u,v}$ is isomorphic to $\mathsf{A}_{\mathsf{MZV}}$ as commutative algebras, one can define a coaction on $C_{u,v}$ by transport of structure. What does this look like in the basis of $C_{u,v}$? This interesting question, not obvious at all, is not considered in this article. In relation to the next paragraph, it may be useful for this purpose to understand first the motivic coaction on arborified multiple zeta values.

The two special cases with parameters u, v being $(1, 0)$ or $(0, 1)$ are specially interesting, as the conjectural bases obtained are then made of some arborified multiple zeta values, as studied in [16, 7, 19]. Another interesting value could be $(1, 1)$, in relation with the multiple zeta-star values as defined and studied in [18, 13]. Indeed, in this case, the conjectural basis in weight 3 consists of the element $\zeta(1, 2) + \zeta(3)$, which is the multiple zeta-star value $\zeta^*(1, 2)$.

The construction of the sub-algebras $C_{u,v}$ is rather simple, as the zinbiel sub-algebras generated inside $\mathsf{A}_{1,0}$ by two chosen elements z_2 and z_3 in degrees 2

and 3. To show that they have the correct dimensions, one just needs to prove that they are free as zinbiel algebras. Similar results about freeness of zinbiel sub-algebras of free zinbiel algebras have been obtained in [17].
It is possible that the same kind of ideas could be applied to some variants of multiple zeta values, in particular to the alternating multiple zeta values.

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2 Zinbiel algebras

Some references on zinbiel algebras are [14, 8, 15].
A zinbiel algebra over a commutative ring R is a module L over R endowed with a bilinear product $\prec : L \otimes_R L \to L$ such that

$$(x \prec y) \prec z = x \prec (y \prec z) + x \prec (z \prec y) \tag{1}$$

for all x, y, z in L. This implies the symmetry

$$(x \prec y) \prec z = (x \prec z) \prec y.$$

It is then convenient to introduce the symmetrized product ш defined by

$$x \,ш\, y = x \prec y + y \prec x, \tag{2}$$

for x, y in L. It can be deduced from (1) that ш is always a commutative and associative product on L.
We will always denote by $\prec$ the zinbiel product in a zinbiel algebra.
By general algebraic arguments, one can define abstractly the free zinbiel algebra $\mathrm{Zin}(S)$ over a set S by its universal property: any morphism of sets from S to a zinbiel algebra L can be uniquely extended to a morphism of zinbiel algebras from $\mathrm{Zin}(S)$ to L.
The free zinbiel algebra on a finite set S over a field k has a very neat and simple explicit description. The underlying vector space has a basis indexed by non-empty words with letters in S. The zinbiel product of two words w and w' is the sum of words in the standard shuffle product of w and w' in which the first letter comes from the first letter of w. Here is one way to remember this rule: the symbol $\prec$ is pointing towards the word whose first letter remains the first letter.
For example, for $s \in S$ and w a word, $s \prec w$ is just the word sw. For $s, t, u \in S$, one finds that $st \prec u = stu + sut$.

Let us introduce a notation for the right-parenthesized zinbiel product. Let $a_1, \dots, a_n$ be elements of a zinbiel algebra. If $n = 1$, let $\mathsf{K}(a_1) = a_1$. Otherwise, define by induction

$$\mathsf{K}(a_1, \dots, a_n) = a_1 \prec \mathsf{K}(a_2, \dots, a_n). \tag{3}$$

In the free zinbiel algebra over a finite set S, the basis element indexed by a word $(s_1, \dots, s_n)$ with letters in S is exactly $\mathsf{K}(s_1, \dots, s_n)$.
When using the commutative algebra $(Z, ш)$ associated with a free zinbiel algebra $(Z, \prec)$, one has to be cautious about units, as the empty word ε is not in the basis of Z. We will abuse notation and assume implicitly that, whenever required, one uses instead of $(Z, ш)$ the unital commutative algebra $(Z \oplus \mathbb{Q}\varepsilon, ш)$ where the empty word ε is the added unit.

3 Algebra of convergent words in 0, 1

Let A be the free zinbiel algebra on two generators 0 and 1.
By the general description of free zinbiel algebras recalled above, A has a basis indexed by non-empty words in $0, 1$. In this basis, the product $\prec$ is one-half of the shuffle product. For example,

$$(\mathbf{1}0) \prec (10) = (\mathbf{1}010) + 2(\mathbf{1}100),$$

where we have emphasized the letter that remains the first letter. The associated commutative product ш is the standard shuffle product.
The algebra A is bigraded, by the number of 0's and the number of 1's in a word.
Let $\mathscr{A}_{1,0}$ be the set of words starting with 1 and ending with 0. Let $\mathsf{A}_{1,0}$ be the sub-space of A spanned by these words. Then clearly $\mathsf{A}_{1,0}$ is a zinbiel sub-algebra of A.
The algebra $\mathsf{A}_{1,0}$ is not a free zinbiel algebra, because of the following relations. For every pair of words x and y in $\mathscr{A}_{1,0}$, there holds

$$(1x) \prec y = (1y) \prec x. \tag{4}$$

Indeed, when seen in A, this equality becomes

$$(1 \prec x) \prec y = (1 \prec y) \prec x,$$

which is a consequence of the zinbiel axiom (1).

4 Free sub-algebras

Our aim is to build, inside the algebra $\mathsf{A}_{1,0}$, free zinbiel sub-algebras on two generators.
More precisely, let u and v be two parameters, not both zero and define

$$z_2 = (1, 0) \quad \text{and} \quad z_3 = u(1, 0, 0) + v(1, 1, 0) \tag{5}$$

in $\mathsf{A}_{1,0}$.
Let $C_{u,v}$ be the zinbiel sub-algebra of $\mathsf{A}_{1,0}$ generated by z_2 and z_3. Note that it only depends on the class of (u, v) in the projective line $\mathbb{P}^1$.
As both z_2 and z_3 are homogeneous with respect to the total grading of $\mathsf{A}_{1,0}$ by the length of words, $C_{u,v}$ inherits a grading where z_2 has degree 2 and z_3 has degree 3.
For a word $w = (w_1, \dots, w_n)$ in the alphabet $\{2, 3\}$, let us denote

$$\mathsf{K}_{u,v}(w) = \mathsf{K}(z_{w_1}, \dots, z_{w_n}). \tag{6}$$

The degree of $\mathsf{K}_{u,v}(w)$ is the sum of the letters of w.

Theorem 1. *For all (u, v) not both zero, the sub-algebra $C_{u,v}$ is a free zinbiel algebra on the two generators z_2, z_3 over $\mathbb{Q}$.*

Proof. Using the grading of $C_{u,v}$, it is enough to fix a degree d and prove that the elements $K_{u,v}(w)$ for all words w in 2 and 3 of sum d are linearly independent in $\mathsf{A}_{1,0}$. By using the bigrading of $\mathsf{A}_{1,0}$, one can instead prove the linear independence of the leading terms of these elements $K_{u,v}(w)$ with respect to either grading. By leading term, one means here and below the homogeneous component of highest degree.
If $u \neq 0$, the leading term of $K_{u,v}(w)$ with respect to the number of 0's is a non-zero multiple of the element $K_{1,0}(w)$.
If $v \neq 0$, the leading term of $K_{u,v}(w)$ with respect to the number of 1 is a non-zero multiple of the element $K_{0,1}(w)$.
It is therefore enough to prove the statement in the cases $(u, v) = (1, 0)$ and $(u, v) = (0, 1)$. This is done in the next two sections, using a rather standard strategy. □

Note that these two cases are really distinct, as there is no zinbiel automorphism of $\mathsf{A}_{1,0}$ that would exchange them.

Lemma 1. *Let w_1, w_2, …, w_n be words in $\mathsf{A}_{1,0}$. Then $\mathsf{K}(w_1, \dots, w_n)$ is the sum over all shuffles of the words w_i such that the first letters remain in the same order.*

In this statement, shuffles are permutations of the positions of letters in the concatenation of w_1, w_2, …, w_n. The statement is easily proved by induction, starting from the definition of $\prec$.
These shuffles will be called good-shuffles. The identity shuffle, corresponding to the concatenation of words, is always a good-shuffle.

4.1 Words 10 and 100

Let $C_{10,100}$ be the zinbiel sub-algebra of $\mathsf{A}_{1,0}$ generated by the words 10 and 100. Let us denote in this section the word 10 by 2 and the word 100 by 3. The algebra $C_{10,100}$ is bigraded by the number of 2 and the number of 3, as 10 and 100 are homogeneous in $\mathsf{A}_{1,0}$ with linearly independent bidegrees.

For a word w in the alphabet $\{2, 3\}$, let $\mathbf{cat}\, w$ be the word in $\mathsf{A}_{1,0}$ obtained from w by the substitution $2 \mapsto 10$ and $3 \mapsto 100$.
By Lemma 1, for a word $w = w_1 \dots w_n$ in $\{2, 3\}$, the expansion of $\mathsf{K}(w) = \mathsf{K}(w_1, \dots, w_n)$ is a sum of words in $\{0, 1\}$ with the following property: the letters 1 (one in each w_i) remain in the same order. Moreover, every letter 0 coming from w_i is placed somewhere on the right of the letter 1 coming from w_i. In this case, we will say that these 0's are associated with this 1.

Theorem 2. *The zinbiel algebra $C_{10,100}$ is free over $\mathbb{Z}$.*

Proof. Because $C_{10,100}$ is generated by 2 and 3, its dimensions are bounded above by the dimensions of the free zinbiel algebra in two generators.
It is therefore enough to prove that the dimension of the homogeneous component of any given bidegree (k, ℓ) with respect to 2 and 3 is at least the number of words with k letters 2 and ℓ letters 3.
Let us fix (k, ℓ) and consider the set S of words with k letters 2 and ℓ letters 3. Let us endow S with the lexicographic order induced by the ordering of letters $2 < 3$.
Let M be the square matrix with rows and columns indexed by S with coefficient $M_{w,w'}$ being the number of occurrences of the word $\mathbf{cat}\, w'$ in the expansion of $\mathsf{K}(w)$ as a sum of words in $\{0, 1\}$.
Let us prove that M is upper triangular with 1 on the diagonal.

Lemma 2. *Let $w, w' \in S$ such that $M_{w,w'} \neq 0$ and w shares a prefix with w'. Then the restriction to the common prefix of any good-shuffle that maps $\mathbf{cat}\, w$ to $\mathbf{cat}\, w'$ is the identity.*

Proof. This is proved by induction on the length i of the common prefix, starting from the empty prefix. Let us assume the induction hypothesis before w_i and that moreover $w_i = w'_i$. The 1 in w'_i must come from the 1 in w_i because the 1's remain in the same order. Then the 0's (one or two) in w'_i must be to the right of their associated 1, which must therefore be the 1 coming from w_i, as the previous 1's are already followed immediately by all their associated 0's. The only possible way is that the 0's in w'_i are not shuffled and remain at their initial positions in w_i. □

In the case $w = w'$, this lemma implies that the diagonal of M is made of 1's. Now consider $w \neq w' \in S$ such that $M_{w,w'} \neq 0$ and the first different letter happens at position i, where $w_i \neq w'_i$. One has to prove that w' is before w in the lexicographic order. Assume by contradiction that $w_i = 2$ and $w'_i = 3$. By the lemma 2, any good-shuffle that maps $\mathbf{cat}\, w$ to $\mathbf{cat}\, w'$ is the identity on the common prefix of w and w'. Therefore the letter 1 in w'_i comes from the letter 1 in w_i and has only one associated 0. But then the two 0's in w'_i need to have their associated 1 on their left, which is not possible. Indeed, the 1's in the common prefix are already followed immediately by all their associated 0's, and the 1 in w'_i has only one associated 0. □

To illustrate the proof, here is the case of words w with one 2 and two 3:

$$\begin{aligned}
\mathsf{K}(2,3,3) &= (10100100) + \dots,\\
\mathsf{K}(3,2,3) &= 2(10100100) + (10010100) + \dots,\\
\mathsf{K}(3,3,2) &= 6(10100100) + 2(10010100) + (10010010) + \dots,
\end{aligned}$$

where on the right only words of the form $\mathbf{cat}\, w'$ have been displayed.

4.2 Words 10 and 110

Let us now turn to the other case, slightly more complicated.
Let $C_{10,110}$ be the zinbiel sub-algebra of $\mathsf{A}_{1,0}$ generated by the words 10 and 110. Let us denote in this section the word 10 by 2 and the word 110 by 3. The algebra $C_{10,110}$ is bigraded by the number of 2 and the number of 3, as 10 and 110 are homogeneous in $\mathsf{A}_{1,0}$ with linearly independent bidegrees.
For a word w in the alphabet $\{2, 3\}$, let $\mathbf{cat}\, w$ be the word in $\mathsf{A}_{1,0}$ obtained from w by the substitution $2 \mapsto 10$ and $3 \mapsto 110$.

Theorem 3. *The zinbiel algebra $C_{10,110}$ is free over $\mathbb{Q}$.*

Proof. Because $C_{10,110}$ is generated by 2 and 3, its dimensions are bounded above by the dimensions of the free zinbiel algebra in two generators.
It is therefore enough to prove that the dimension of the homogeneous component of any given bidegree (k, ℓ) with respect to 2 and 3 is at least the number of words with k letters 2 and ℓ letters 3.
Let us fix (k, ℓ) and consider the set S of words with k letters 2 and ℓ letters 3. Let us endow S with the lexicographic order induced by the ordering of letters $2 < 3$.
Let M be the square matrix with rows and columns indexed by S with coefficient $M_{w,w'}$ being the number of occurrences of the word $\mathbf{cat}\, w'$ in the expansion of $\mathsf{K}(w)$ as a sum of words in $\{0, 1\}$.
Let us prove that M is lower triangular with no zero on the diagonal.
Let us first remark that the diagonal coefficient for a word w in S counts the number of good-shuffles that preserves $\mathbf{cat}\, w$. But this set always contains the identity shuffle, hence every diagonal coefficient of M is a non-zero integer.

Lemma 3. *Let $w, w' \in S$ such that $M_{w,w'} \neq 0$ and w shares a prefix $w_1 \dots w_i$ with w'. Let σ be any good-shuffle that maps $\mathbf{cat}\, w$ to $\mathbf{cat}\, w'$. Then*

(i) either σ stabilizes the common prefix,

(ii) or the following statements hold:

- There exists a letter 3 in the prefix. Let w_k be the rightmost such letter. The shuffle σ stabilizes the prefix before w_k.

- The letter w_{i+1} is 2.

- *Between w_k and w_{i+1}, the shuffle σ acts in the following way:*

$$\begin{array}{rr|rrcr|r} & \dots & w_k = 3 & 2 & \dots & w_i = 2 & w_{i+1} = 2 \\ w & \dots & \underline{1}10 & 10 & \dots & 10 & 10 \\ w' & \dots & \underline{1}10 & 10 & \dots & 10 & \end{array}$$

The first letter $\underline{1}$ of w_k is sent to the first letter $\underline{1}$ of w'_k. Each block 10 *(from a letter* 2*) displayed in the line w above is sent leftwards to the block* 10 *(from w_k or a letter* 2*) in the previous term of the line w'. The block* 10 *inside w_k is sent rightwards somewhere in the suffix of w' after w'_i.*

Proof. This is proved by induction on the length of the common prefix, starting with the empty prefix.
Assume first the induction hypothesis with condition (i) before w_i and moreover $w_i = w'_i$. Necessarily, the first 1 in w'_i must come from the first 1 in w_i, as the order is preserved on the first letters.
If w_i is 2, the 0 in w'_i must come from the 0 in w_i, as the only available 1 to its left is that of w'_i. So condition (i) holds for the extended prefix.
If w_i is 3, and if the second 1 in w'_i comes from w_i too, one finds that condition (i) holds for the extended prefix, for the same reason as in the previous case.
Otherwise, the second 1 in w'_i must come from w_{i+1}. And the 0 in w'_i must be preceded by all the associated 1's. This implies that this 0 comes from w_{i+1} and that $w_{i+1} = 2$. All this gives condition (ii) for the extended prefix, in the special situation where $k = i$.
Assume now the induction hypothesis with condition (ii) before w_i and moreover $w_i = w'_i$. Then w_i is a 2.
Assume first that σ sends the second 1 of w_k to the 1 in w'_i. Then the 0 in w_k must be sent to the 0 in w'_i. Therefore in this case, one obtains condition (i) for the extended prefix.
Otherwise, σ sends the second 1 of w_k somewhere in the suffix of w' after w'_i. Then the first 1 of w_{i+1} must be sent to the first one of w'_i. And the 0 in w'_i must be preceded by all the associated 1's. This implies that this 0 comes from w_{i+1} and that $w_{i+1} = 2$.
The first statement of condition (ii) holds by induction. We just proved the two other statements, so condition (ii) holds for the extended prefix. □

Now consider $w \neq w' \in S$ such that $M_{w,w'} \neq 0$ and the first different letter happens at position i where $w_i \neq w'_i$. One has to prove that w' is after w in the lexicographic order. Assume by contradiction that $w_i = 3$ and $w'_i = 2$. Let σ be any good-shuffle that maps $\mathbf{cat}\, w$ to $\mathbf{cat}\, w'$.
By the lemma 3, either condition (i) or condition (ii) holds for σ.
Condition (ii) cannot hold because $w_i = 3$.
Therefore condition (i) holds. The unique letter 1 in w'_i comes from the first letter 1 in w_i. But then the 0 in w'_i either comes from $w_i = 3$ or from some w_j with $j > i$. In both cases, this 0 has not enough 1's on its left. □

To illustrate the proof, here is the case of words w with one 2 and two 3:

$$\mathsf{K}(2,3,3) = 3(11011010) + (11010110) + (10110110) + \dots,$$
$$\mathsf{K}(3,2,3) = 4(11011010) + 2(11010110) + \dots,$$
$$\mathsf{K}(3,3,2) = 2(11011010) + \dots,$$

where on the right only words of the form $\mathbf{cat}\, w'$ have been displayed.

Remark: One can deduce from the proof of lemma 3 a more precise description of the diagonal coefficients of the matrix M. The coefficient of a word w in 2 and 3 is the product of the lengths of the blocks in the unique factorization of w into blocks $322\dots2$, omitting the possible initial sequence of 2. For example, for $(2,3,3,2,3,2)$, one gets $4 = 1 \times 2 \times 2$.

4.3 Remarks and questions

One could ask the same question of freeness about several larger zinbiel sub-algebras of $\mathsf{A}_{1,0}$.

Sometimes the answer is clearly negative, for the same reasons as for $\mathsf{A}_{1,0}$. This is for instance the case of the sub-algebra generated by the words $10, 110, 1110$ in which the relation $110 \prec 110 = 1110 \prec 10$ holds, as a special case of (4).

The following cases may be free, as these algebras do not contain any obvious relation of this kind. Let U be the set of words of the shape $10\dots0$, with just one letter 1.

(A) the sub-algebra generated by words $10, 100, 110$,

(B) the sub-algebra generated by words in U,

(C) the sub-algebra generated by 110 and words in U,

(D) the sub-algebra generated by words not starting with 11,

(E) the sub-algebra generated by 110 and words not starting with 11.

Some closely related questions have been answered in [17, §4].

5 Quotient map to motivic multiple zeta values

We will use the following convention for formal iterated integrals:

$$I(\varepsilon_1,\dots,\varepsilon_k) = \int\cdots\int_{0<t_1<\dots<t_k<1} \omega_{\varepsilon_1}(t_1)\cdots\omega_{\varepsilon_k}(t_k), \tag{7}$$

where each ε_i is either 0 or 1, with $\varepsilon_1 = 1$ and $\varepsilon_k = 0$.

We will denote motivic multiple zeta values $\zeta(n_1,\dots,n_k)$, with the convention

$$\zeta(k_1,\dots,k_r) = I(1,0^{k_1-1},1,0^{k_2-1},\dots,1,0^{k_r-1}) \tag{8}$$

for $r \geq 1$. Here a power of 0 means a repeated 0.
Let us denote by Π the surjective quotient morphism of commutative algebras from $\mathsf{A}_{1,0}$ to $\mathsf{A}_{\mathsf{MZV}}$, whose kernel is the ideal of motivic relations between formal iterated integrals. The shuffle product ш on $\mathsf{A}_{1,0}$ is sent by Π to the product of motivic multiple zeta values.
For (u, v) not both zero, the space $C_{u,v}$ is a zinbiel sub-algebra of $\mathsf{A}_{1,0}$, hence also a commutative sub-algebra of $\mathsf{A}_{1,0}$ for the symmetrized product, which is just the shuffle product.
For every choice of parameters (u, v) not both zero, one can therefore restrict Π to this commutative sub-algebra $C_{u,v}$ of $\mathsf{A}_{1,0}$. This gives a morphism of commutative graded algebras Π from $C_{u,v}$ to $\mathsf{A}_{\mathsf{MZV}}$. Note that these two graded algebras have the same generating series $F = 1/(1 - x^2 - x^3)$.
One can therefore wonder if the morphism Π could be an isomorphism, under some conditions on (u, v). As the algebra $C_{u,v}$ itself, this property only depends on the projective class of (u, v) in $\mathbb{P}^1$.
Let us consider first the very special case where $u + v = 0$. In this case, the image of the word z_3 in $C_{u,v}$ is given by $\Pi(z_3) = u\zeta(3) + v\zeta(1, 2)$. But it is known that $\zeta(3) = \zeta(1, 2)$ in $\mathsf{A}_{\mathsf{MZV}}$, hence $\Pi(z_3) = 0$. Therefore Π is not surjective in this case.
Using a computer, one can compute the first few graded dimensions of the image.

Conjecture 1. *When $u + v = 0$, the image of $C_{u,v}$ by Π is a sub-algebra of $\mathsf{A}_{\mathsf{MZV}}$ with generating series $1 + x^2 F$.*

This is the generating series of the quotient algebra of $\mathsf{A}_{\mathsf{MZV}}$ by $\zeta(3)$, because

$$1 + x^2 F = (1 - x^3)F. \tag{9}$$

One can wonder what could be, for this sub-algebra, an analog of the famous conjecture of Broadhurst-Kreimer describing the dimensions of $\mathsf{A}_{\mathsf{MZV}}$ according to both weight and depth.
Note also the similarity with the quotient algebra of $\mathsf{A}_{\mathsf{MZV}}$ by $\zeta(2)$, which has generating series

$$1 + x^3 F = (1 - x^2)F \tag{10}$$

and appears in the motivic coaction and in the study of p-adic multiple zeta values [9, 10].

Excluding from now on the special case $u + v = 0$, one can assume without loss of generality that $u + v = 1$ and set $v = 1 - u$. Then $\Pi(z_3) = \zeta(3)$.
When using u as a formal parameter, one expects the following statement.

Conjecture 2. *The morphism Π from $C_{u,1-u}$ to $\mathsf{A}_{\mathsf{MZV}}$ is generically an isomorphism of commutative algebras.*

In this statement, the word “generic” means over the field $\mathbb{Q}(u)$. One could instead ask for the statement to hold for u in some open subset of $\mathbb{Q}$ with respect to the complex topology. One probably cannot expect an open set for the Zariski topology on $\mathbb{Q}$, because the following explanations tend to exclude an infinite set.

Let us say that a value of u is NON-SINGULAR if this statement holds at u, and SINGULAR otherwise. If there exists at least one non-singular value, then the generic conjecture 2 also holds.

For every non-singular u, the isomorphism Π defines a bigrading of the algebra $\mathsf{A}_{\mathsf{MZV}}$. Moreover, one gets a basis in $\mathsf{A}_{\mathsf{MZV}}$ from the basis of $C_{u,1-u}$ made of words in z_2 and z_3.

More and more singular values appear when considering the restriction of Π at increasing weights. In each weight, a new polynomial determinant appears, with some irreducible factors coming from determinants in lower weights. One observes new irreducible factors of increasing degrees, that give more singular values, so that one should expect an infinite number of singular values. One could still hope that some specific values of u are non-singular, for example $u = 0$ and $u = 1$. So far, no non-singular value of u is known.

Let us describe the first few polynomials whose zeroes are singular values, in their order of apparition, where n is the weight.

n	p_n
5	$5u - 6$
7	$14u + 51$
8	$27u^2 - 26u + 10$
9	$865u - 4164$
10	$2011u^2 - 3381u + 1581$
11	$461516u^4 - 3721029u^3 + 7046644u^2 - 6169912u + 2357966$
12	$207786u^4 - 185687u^3 - 1076020u^2 + 1483088u - 562680$

One can check that 0 and 1 are not roots of any of these polynomials.

Let us comment briefly on how these polynomials were computed. The idea is to compute, for a fixed weight d, the determinant of a square matrix that is invertible if and only if Π is an isomorphism. One first computes the images by Π of all words in z_2 and z_3 of weight d in $\mathsf{A}_{\mathsf{MZV}}$. Then, instead of computing their coefficients in some known basis of $\mathsf{A}_{\mathsf{MZV}}$, one uses the isomorphism[1], introduced by F. Brown [6], from the algebra $\mathsf{A}_{\mathsf{MZV}}$ to the shuffle algebra F in infinitely many generators $f_3, f_5, f_7, f_9, \dots$ over the polynomial ring $\mathbb{Q}[f_2]$. This algebra F has a natural basis, and we use this basis to form the desired matrix. An example is given below.

Let us give the first few images by the morphism Π from $C_{u,1-u}$ to $\mathsf{A}_{\mathsf{MZV}}$ of short words in z_2 and z_3.

[1]This useful isomorphism is not unique and depends on some auxiliary choices.

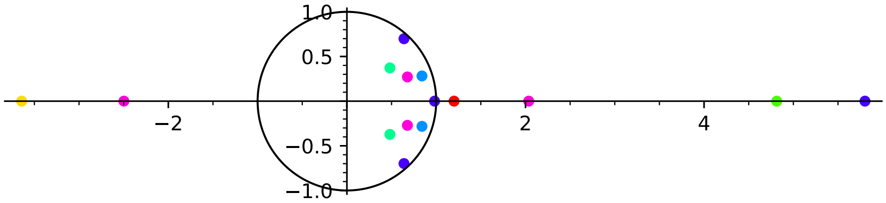

Figure 1: Singular values of u in weight at most 12. The point near 1 is the root $0.98188\ldots$ of p_{11} and the point near 2 is the root $2.03611\ldots$ of p_{12}.

$$B(2) = \zeta(2), \tag{11}$$
$$B(3) = \zeta(3), \tag{12}$$
$$B(2,2) = 2\zeta(1,3) + \zeta(2,2), \tag{13}$$
$$B(2,3) = (u+2)\,\zeta(1,4) + \zeta(2,3) + (-u+1)\,\zeta(3,2), \tag{14}$$
$$B(3,2) = (-u+4)\,\zeta(1,4) + 2\zeta(2,3) + u\zeta(3,2). \tag{15}$$

One can then check that $B(2)B(3) = B(2,3) + B(3,2)$, as a simple example of the general rule that the product in the conjectural bases is given by the shuffle product.

The motivic coaction Δ (modulo $\zeta(2)$ on the left side of $\otimes$) is given on these elements by

$$\begin{aligned}
\Delta B(2) &= 1 \otimes B(2),\\
\Delta B(3) &= 1 \otimes B(3) + B(3) \otimes 1,\\
\Delta B(2,2) &= 1 \otimes B(2,2),\\
\Delta B(2,3) &= 1 \otimes B(2,3) + (u-1)B(3) \otimes B(2) + B(2,3) \otimes 1,\\
\Delta B(3,2) &= 1 \otimes B(3,2) + (-u+2)B(3) \otimes B(2) + B(3,2) \otimes 1.
\end{aligned}$$

In weight 5, the images of $B(2,3)$ and $B(3,2)$ in the algebra F are

$$(u-1)f_2f_3 - (5/2u-3)f_5 \quad \text{and} \quad (-u+2)f_2f_3 + (5/2u-3)f_5,$$

from which one builds a square matrix with determinant proportional to $5u-6$.

6 Variants of multiple zeta values

There are some other situations where one could try to apply the same ideas. A first example is given by the algebra of alternating multiple zeta values, defined as the iterated integrals of the following three 1-forms:

$$\omega_0 = \frac{dt}{t}, \omega_{-1} = \frac{dt}{t-1}, \omega_1 = \frac{dt}{t+1}. \tag{16}$$

A conjecture due to Broadhurst (see [1, 2]) states that the graded dimensions of this algebra are given by the Fibonacci numbers, with generating series $1/(1-x-x^2)$.
One could therefore consider the zinbiel sub-algebra of the free zinbiel algebra on $\{-1,0,1\}$ generated by the abstract iterated integrals $I(-1)$ and $I(1,0)$. Is this a free zinbiel algebra on these generators ?

A similar case is the algebra of multiple Landen values, defined in [3] as iterated integrals of the following 1-forms: $A = dx/x$, $B = dx/(1-x)$, $F = dx/(1-\rho^2 x)$ and $G = dx/(1-\rho)$ where ρ is the golden ratio.
Broadhurst conjectured in [3] that the generating series for this algebra is $1/(1-x-x^2-x^3)$, whose coefficients are tribonacci numbers. The exact same formula is also expected to give the graded dimensions of the sub-algebra of iterated integrals of A and G.
The first few terms are

$$1, 1, 2, 4, 7, 13, 24, 44, 81, 149, 274, 504, 927, 1705, \dots$$

and the expected bases, as words in A and G are $\{G\}$ in degree 1; $\{AG, GG\}$ in degree 2 and $\{AGG, AAG, GAG, GGG\}$ in degree 3.
In this setting, one could look for a free zinbiel sub-algebra on three generators of degrees $1, 2$ and 3 inside the free zinbiel algebra on A and G.
Another interesting case to consider would be multiple Watson values [4].

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