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Algebra of Multiple Zeta Values: Harmonic and Shuffle Products

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Multiple Zeta Values

For positive integers $i_1, i_2, \ldots i_k$ with $i_1 > 1$, we define multiple zeta values (henceforth MZVs) by

$$\zeta(i_1, i_2 \ldots, i_k) = \sum_{n_1 > n_2 \cdots > n_k \geq 1} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}}.$$

We call k the length of the series, and $i_1 + \cdots + i_k$ its weight. Of course, if the length is 1 the MZVs are the values $\zeta(i)$ of the Riemann zeta function at positive integers $i > 1$.

Coding MZVs

The following coding scheme is remarkably useful. Associate to each sequence $(i_1, \ldots, i_k)$ the word $x^{i_1-1}yx^{i_2-1}y \cdots x^{i_k-1}y$ in noncommuting variables x and y. For example:

$$(2) \leftrightarrow xy, \quad (3,2,1,1) \leftrightarrow x^2yxy^3$$

Every admissible sequence $(i_1, \ldots, i_k)$ (one with $i_1 > 1$) corresponds to an admissible word w (one that that begins with x and ends with y); we can think of ζ as assigning a real value to every such word. (It is convenient to treat the empty word 1 as admissible and set $\zeta(1) = 1$.) The length k of the sequence is the y-degree of w (denoted $\ell(w)$), and the weight $i_1 + \cdots + i_k$ of the sequence is the total degree $|w|$ of w.

The Duality Theorem

The coding scheme gives a striking way to state a class of identities for MZVs which we call the Duality Theorem. Let τ be the order-reversing function on words that exchanges x and y (so $\tau(x^2yxy) = xyxy^2$).

Duality Theorem

For any admissible word w, $\zeta(w) = \zeta(\tau(w))$.

For example,

$$\zeta(3,2,1,1) = \zeta(x^2yxy^3) = \zeta(x^3yxy^2) = \zeta(4,2,1).$$

Duality Theorem cont'd

Proof.

If we define iterated integrals by $\int_0^t \alpha_1 = \int_0^t f(s)ds$ and

$$\int_0^t \alpha_1\alpha_2\cdots\alpha_n = \int_0^t f(s)\left(\int_0^s \alpha_2\cdots\alpha_n\right)ds$$

for $\alpha_1 = f(t)dt$, then it is straightforward to show that

$$\zeta(x^{p_1}y\cdots x^{p_l}y) = \int_0^1 \alpha^{p_1}\beta\cdots\alpha^{p_l}\beta,$$

where $\alpha = dt/t$ and $\beta = dt/(1-t)$. The theorem then follows from the change of variable $(t_1,\ldots,t_n) \to (1-t_n,\ldots,1-t_1)$. $\square$

Derivation Theorem

In an early attempt to prove the Duality Theorem, I managed to prove something else (Hoffman, 1992). If we let $\mathfrak{H}^0$ be the rational vector space whose basis is the set of admissible words, then ζ extends linearly to a map $\mathfrak{H}^0 \to \mathbf{R}$, and τ to a map $\mathfrak{H}^0 \to \mathfrak{H}^0$. Also, define $D(x) = 0$, $D(y) = xy$, and extend D to $\mathfrak{H}^0$ as a derivation (of $\mathfrak{H}^0$ as a subalgebra of $\mathbf{Q}\langle x, y\rangle$).

Derivation Theorem

For all admissible words w, $\zeta(D(w)) = \zeta(D\tau(w))$.

My proof of this used partial fractions. But perhaps the greater significance of this result is that it showed the utility of the x, y coding scheme goes beyond its correspondence with the iterated integral representation.

Sum Theorem

Much of the early work on MZVs (including my own) was motivated by attempts to prove the following result.

Sum Theorem

For $n \geq 2$ and fixed $k < n$,

$$\sum_{w \in \mathfrak{H}^0, |w|=n, \ell(w)=k} \zeta(w) = \zeta(n).$$

This result was proved by Granville and Zagier (independently) in 1995, and has since been generalized in several ways. One such generalization was obtained by Y. Ohno in 1999; his result generalizes the Duality and Derivation Theorems as well. We will state Ohno's Theorem in our second lecture.

Algebraic Structures on $\mathfrak{H}^0$

There are two important algebraic structures on MZVs that we will consider.

1. The shuffle algebra $(\mathfrak{H}^0, \sqcup\!\sqcup)$, corresponding to the iterated integral representation mentioned above.
2. The harmonic algebra $(\mathfrak{H}^0, *)$, based on the multiplication of series. $(\mathfrak{H}^0, *)$ is a subalgebra of the algebra QSym of quasi-symmetric functions.

The Shuffle Algebra

Let $\mathfrak{H}$ be $\mathbf{Q}\langle x, y\rangle$ as a graded rational vector space. Define a multiplication $\sqcup\!\sqcup$ on $\mathfrak{H}$ by requiring that it distribute over the addition, and that it satisfy the following axioms:

S1. for any word w, $1 \sqcup\!\sqcup w = w \sqcup\!\sqcup 1 = w$;

S2. for any words w_1, w_2 and letters a, b,

$$aw_1 \sqcup\!\sqcup bw_2 = a(w_1 \sqcup\!\sqcup bw_2) + b(aw_1 \sqcup\!\sqcup w_2).$$

Induction on word length establishes the following.

Theorem

The $\sqcup\!\sqcup$-product is commutative and associative.

Shuffle Algebra cont'd

There is a familiar presentation of the shuffle product in terms of permutations: let $S(n)$ be the symmetric group on n letters, and for positive integers k, l such that $k + l = n$ define $S(k, l)$ as the set of $\sigma \in S(n)$ such that

$$\sigma(1) < \cdots < \sigma(k) \quad \text{and} \quad \sigma(k+1) < \cdots < \sigma(k+l).$$

Then for letters $a_1, \ldots, a_n$,

$$a_1 \cdots a_k \sqcup\!\sqcup a_{k+1} \cdots a_{k+l} = \sum_{\sigma \in S(k,l)} a_{\sigma(1)} \cdots a_{\sigma(n)}.$$

This description makes the following fact evident.

Theorem

τ is an automorphism of $(\mathfrak{H}, \sqcup\!\sqcup)$.

Lyndon Words

Order the words of $\mathfrak{H}$ as follows. For any words w_1, w_2, w_3, set $w_1 x w_2 < w_1 y w_3$; and if u, v are words with v nonempty, set $u < uv$. A nonempty word w of $\mathfrak{H}$ is called a Lyndon word if it is smaller than any of its nontrivial right factors; i.e., $w < v$ whenever $w = uv$ and $u \neq 1 \neq v$. For example, the Lyndon words of degree ≤ 4 are

$$x, y, xy, x^2y, xy^2, x^3y, x^2y^2, xy^3.$$

From (Radford, 1979) we have

Theorem

As a commutative algebra, $(\mathfrak{H}, ⧢)$ is freely generated by the Lyndon words.

Shuffle Identities

The link to MZVs is the following result, which follows from the iterated-integral representation mentioned before, together with the well-known fact (Ree, 1957) that iterated integrals multiply by shuffle product.

Theorem (Shuffle Homomorphism)

The map $\zeta : (\mathfrak{H}^0, ⧢) \to \mathbf{R}$ *is a* τ*-equivariant homomorphism.*

The shuffle-algebra structure has been used to prove some MZV identities. For example, Borwein, Bradley, Broadhurst and Lisoněk (1998) first establish that

$$\sum_{r=-n}^{n} (-1)^r [(xy)^{n-r} ⧢ (xy)^{n+r}] = 4^n (x^2 y^2)^n$$

Shuffle Identities cont'd

in $(\mathfrak{H}, ⧢)$, then apply ζ to get

$$\sum_{r=-n}^{n} (-1)^r \zeta((xy)^{n-r})\zeta((xy)^{n+r}) = 4^n \zeta((x^2y^2)^n).$$

Using the known result

$$\zeta((xy)^k) = \frac{\pi^{2k}}{(2k+1)!} \tag{1}$$

(of which more later) together with some arithmetic, they obtain a result conjectured by Zagier some years earlier:

$$\zeta((x^2y^2)^n) = \frac{1}{2n+1}\zeta((xy)^{2n}).$$

Other shuffle convolutions are used to prove instances of the "cyclic insertion conjecture" for MZVs in the same paper. The topic has been revisited by Bowman and Bradley (2002).

The Harmonic Algebra

As before, let $\mathfrak{H}$ be $\mathbf{Q}\langle x, y\rangle$ as a rational vector space. Define a commutative multiplication $*$ on $\mathfrak{H}$ by requiring that it distribute over the addition and satisfy the following axioms:

H1. for any word w, $1 * w = w * 1 = w$;

H2. for any word w and integer $n \geq 1$,

$$x^n * w = w * x^n = wx^n;$$

H3. for any words w_1, w_2 and integers $p, q \geq 0$,

$$\begin{aligned} x^p y w_1 * x^q y w_2 &= x^p y(w_1 * x^q y w_2) \\ &\quad + x^{p+q+1} y(w_1 * w_2) + x^q y(x^p y w_1 * w_2). \end{aligned}$$

Note that in (H3) each $*$-product on the right-hand side has fewer factors of y than the $*$-product on the left-hand side, so the $*$-product of any pair of words can be computed inductively.

Harmonic Algebra cont'd

Induction on the y-degree $\ell(w)$ establishes the following result.

Theorem

The $*$-product is commutative and associative.

While τ is *not* an automorphism of the harmonic algebra $(\mathfrak{H}, *)$, we do have counterparts of the results for the shuffle algebra (Hoffman, 1997).

Theorem

As a commutative algebra, $(\mathfrak{H}, *)$ is freely generated by the Lyndon words.

Theorem (Harmonic Homomorphism)

$(\mathfrak{H}^0, *)$ is a subalgebra of $(\mathfrak{H}, *)$, and $\zeta : (\mathfrak{H}^0, *) \to \mathbf{R}$ is a homomorphism.

Comparing the Multiplications $*$ and $ш$

Since the multiplications $*$ and $ш$ differ, The Shuffle Homomorphism and Harmonic Homomorphism Theorems imply that ζ has a large kernel. For example, from

$$\begin{aligned} xy * x^2y &= xyx^2y + x^2yxy + x^4y \\ xy ш x^2y &= xyx^2y + 3x^2yxy + 6x^3y^2. \end{aligned}$$

it follows that

$$\zeta(x^4y - 2x^2yxy - 6x^3y^2) = 0.$$

In fact, the Derivation Theorem can be obtained this way, since

$$y ш w - y * w = \tau D\tau(w) - D(w)$$

for words $w \in \mathfrak{H}^0$.

Harmonic Algebra and QSym

The vector subspace $\mathfrak{H}^1 := \mathbf{Q}1 + \mathfrak{H}y$ of $\mathfrak{H}$ is evidently a subalgebra of $(\mathfrak{H}, *)$. In fact, since x is the only Lyndon word that ends in x, it is easy to see that $\mathfrak{H}^1$ is the subalgebra of $\mathfrak{H}$ generated by the Lyndon words other than x. Note that any word $w \in \mathfrak{H}^1$ is a product of words $z_i = x^{i-1}y$, which are ordered as

$$z_1 > z_2 > \cdots > z_n > \cdots ,$$

and that $\ell(w)$ is its length when expressed this way. In terms of the z_i, the inductive rule for the $*$-product can be written

$$z_p w_1 * z_q w_2 = z_p(w_1 * z_q w_2) + z_q(z_p w_1 * w_2) + z_{p+q}(w_1 * w_2).$$

Now for each positive integer n, define a a map $\phi_n : \mathfrak{H}^1 \to \mathbf{Q}[t_1, \ldots, t_n]$ (where $|t_i| = 1$ for all i) as follows.

Harmonic Algebra and QSym cont'd

Let $\phi_n(1) = 1$ and

$$\phi_n(z_{i_1} z_{i_2} \cdots z_{i_k}) = \sum_{n \geq n_1 > n_2 > \cdots > n_k \geq 1} t_{n_1}^{i_1} t_{n_2}^{i_2} \cdots t_{n_k}^{i_k}$$

for words of length $k \leq n$, and let $\phi(w) = 0$ for words of length exceeding n; extend ϕ_n linearly to $\mathfrak{H}^1$. For any n, ϕ_n is a homomorphism of graded algebras that is injective through degree n. For each $m \geq n$, there is a restriction map

$$\rho_{m,n} : \mathbf{Q}[t_1, \ldots, t_m] \to \mathbf{Q}[t_1, \ldots, t_n]$$

sending t_i to t_i if $i \leq n$ and t_i to 0 if $i > n$. The ϕ_n define a homomorphism ϕ from $\mathfrak{H}^1$ to the inverse limit

$$\mathfrak{P} = \varprojlim_n \mathbf{Q}[t_1, \ldots, t_n]$$

since they commute with restriction.

Harmonic Algebra and QSym cont'd

In fact, $\mathfrak{P}$ is the set of formal power series of bounded degree. Inside $\mathfrak{P}$ is the algebra of symmetric functions

$$\mathrm{Sym} = \varprojlim_n \mathbf{Q}[t_1, \ldots, t_n]^{\Sigma_n}$$

and also the algebra QSym of quasi-symmetric functions, which can be described as follows. A formal series $p \in \mathfrak{P}$ is in QSym if the coefficient of $t_{i_1}^{p_1} \cdots t_{i_k}^{p_k}$ in p is the same as the coefficient of $t_{j_1}^{p_1} \cdots t_{j_k}^{p_k}$ in p whenever $i_1 < \cdots < i_k$ and $j_1 < \cdots < j_k$. Evidently $\mathrm{Sym} \subset \mathrm{QSym}$. A vector space basis for QSym is given by the monomial quasi-symmetric functions

$$M_{(p_1,p_2,\ldots,p_k)} = \sum_{i_1<i_2<\cdots<i_k} t_{i_1}^{p_1} t_{i_2}^{p_2} \cdots t_{i_k}^{p_k},$$

which are indexed by compositions $(p_1, \ldots, p_k)$. Since evidently $\phi(z_{i_1} z_{i_2} \cdots z_{i_k}) = M_{(i_k,\ldots,i_1)}$, we have the following result.

Harmonic Algebra and QSym cont'd

Theorem

ϕ is an isomorphism of $\mathfrak{H}^1$ onto QSym.

As is well known, the algebra Sym of symmetric functions is generated by the elementary symmetric functions e_i, as well as by the power-sum symmetric functions p_i (Note that we are working over $\mathbf{Q}$). It is easy to see that $\phi^{-1}(e_i) = z_1^i = y^i$ and $\phi^{-1}(p_i) = z_i = x^{i-1}y$.
If Sym^0 is the subalgebra of Sym generated by the power-sum symmetric functions p_i with $i \geq 2$, then we have the following result.

Theorem

If $a \in \phi^{-1}(\mathrm{Sym}^0)$, then $\zeta(a)$ is a sum of products of values $\zeta(i)$ of the zeta function with $i \geq 2$.

Harmonic Algebra and QSym cont'd

In fact, to write an MZV corresponding to a symmetric function in terms of values of the zeta function one can write that symmetric function in terms of power-sum symmetric functions p_i and apply ζ. This includes

$$\zeta(z_i^p) = \zeta(i, i, \ldots, i),$$

treated by generating-functions arguments in (Bailey et. al., 1996). For example, since $M_{22} = \frac{1}{2}(p_4 - p_2^2)$ in Sym^0, we have

$$\zeta(2,2) = \frac{1}{2}(\zeta(4) - \zeta(2)^2) = \frac{\pi^4}{120},$$

and more generally equation (1) can be proved this way.