Lectures on Multiple Zeta Values

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CHAPTER 1

The Lure of Multiple Zeta Values

1. Multiple zeta values

The principal source for this lecture is [**7**]. The Riemann zeta function is defined by

$$\zeta(z)=\sum_{n=1}^{\infty}\frac{1}{n^z}$$

for $\Re(z)>1$. It's called the "Riemann" zeta function since Bernhard Riemann (1826-1866) called attention to its properties as a function of a complex variable (and its relevance to the distribution of primes). But a century earlier, Leonhard Euler (1707-1783) had proved some significant results about it, most notably that

$$\zeta(2)=\sum_{n=1}^{\infty}\frac{1}{n^2}=\frac{\pi^2}{6} \tag{1}$$

and more generally

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

where B_{2n} is a Bernoulli number. The first case is equation (1), and the next three are

$$\zeta(4)=\frac{\pi^4}{90},\ \zeta(6)=\frac{\pi^6}{945},\ \zeta(8)=\frac{\pi^8}{9450}.$$

(Euler didn't prove any formula for the values of ζ at the odd integers, and indeed none is known. It was only in 1976 that Roger Apéry (1916-1994) proved $\zeta(3)$ to be irrational; the irrationality of $\zeta(5)$ remains an open question.)

Euler also considered the double series

$$\sum_{i\ge j\ge 1}\frac{1}{i^n j^m},$$

which in modern notation is $\zeta^\star(n,m)=\zeta(n,m)+\zeta(n+m)$. He corresponded about it with Goldbach in 1742-43. Twenty years later Euler returned to this series and wrote a paper about it [**4**]. One of the principal results of that paper is (in modern notation)

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

In 1988, my colleague Courtney Moen got me interested in generalizing this result. Define, for a sequence $a_1,a_2,\dots,a_k$ of positive integers with $a_1\ge 2$, the corresponding multiple zeta value (MZV) by

$$\zeta(a_1,a_2,\dots,a_k)=\sum_{n_1>n_2>\cdots>n_k\ge 1}\frac{1}{n_1^{a_1}n_2^{a_2}\cdots n_k^{a_k}}. \tag{2}$$

We call $a_1 + \cdots + a_k$ the "weight" of the MZV, and k its "depth". Courtney conjectured that the sum of all MZVs of weight n and fixed depth $k \geq 2$ is $\zeta(n)$, independent of k. (We dubbed this the "sum conjecture".) Of course the depth 2 case is Euler's result. Courtney eventually managed to prove the depth 3 case, but his proof was rather long.

Exercise 1. The first case of the sum conjecture is $\zeta(2,1) = \zeta(3)$. Prove it.

I took up the problem in 1988, and immediately noticed that one can multiply MZVs termwise: for example,

$$\zeta(2)\zeta(2) = \sum_{m,n\geq 1} \frac{1}{n^2m^2} = \sum_{m>n\geq 1} \frac{1}{n^2m^2} + \sum_{n=1}^{\infty} \frac{1}{n^4} \sum_{n>m\geq 1} \frac{1}{n^2m^2} = 2\zeta(2,2) + \zeta(4).$$

From this we can conclude that

$$\zeta(2,2) = \frac{1}{2}\left[\zeta(2)^2 - \zeta(4)\right] = \frac{\pi^4}{120}.$$

Exercise 2. Starting with $\zeta(2,1) = \zeta(3)$, prove that

$$2\zeta(2,2,1) + \zeta(2,1,2) + \zeta(4,1) = \zeta(3,2) + \zeta(5)$$

2. Low weights

I started playing around with MZVs of low weight. Here are the MZVs of weights 2 through 6.

$\zeta(2)$

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

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

$\zeta(5),\ \zeta(4,1),\ \zeta(3,2),\ \zeta(2,3),\ \zeta(3,1,1),\ \zeta(2,2,1),\ \zeta(2,1,1,1)$

$\zeta(6),\ \zeta(5,1),\ \zeta(4,2),\ \zeta(3,3),\ \zeta(2,4),\ \zeta(4,1,1),\ \zeta(3,2,1),\ \zeta(3,1,2),\ \zeta(2,3,1),$
$\zeta(2,1,3),\ \zeta(2,2,2),\ \zeta(3,1,1,1),\ \zeta(2,2,1,1),\ \zeta(2,1,2,1),\ \zeta(2,1,1,2),\ \zeta(2,1,1,1,1)$

Exercise 3. Prove that there are $\binom{n-2}{k-1}$ MZVs of weight n and depth k, and hence 2^{n-2} MZVs of weight n.

Now let's look at these low-weight MZVs in more detail. In weight 2 there is just MZV, $\zeta(2)$; by Euler's formula it equals $\frac{\pi^2}{6}$. In weight 3 we have $\zeta(3)$ and $\zeta(2,1)$, but by the relation mentioned above they're equal. In weight 4 we have

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

We've already seen that $\zeta(2,2) = \frac{\pi^4}{120} = \frac{3}{4}\zeta(4)$. Accepting the sum conjecture for depth 2, this means $\zeta(3,1) = \frac{1}{4}\zeta(4)$. What about $\zeta(2,1,1)$? I was able to prove (using an old formula of L. J. Mordell [**10**]) that

$$\zeta(p+1,\underbrace{1,\ldots,1}_{q-1}) = \zeta(q+1,\underbrace{1,\ldots,1}_{p-1}) \tag{3}$$

for $p, q \geq 1$. This implies that $\zeta(2,1,1) = \zeta(4)$.

In weight 5 we have eight MZVs, which we can arrange as follows.

$$\begin{aligned}&\zeta(5)\\&\zeta(4,1),\ \zeta(3,2),\ \zeta(2,3)\\&\zeta(3,1,1),\ \zeta(2,2,1),\ \zeta(2,1,2)\\&\zeta(2,1,1,1)\end{aligned}\tag{4}$$

Now equation (3) gives $\zeta(5)=\zeta(2,1,1,1)$ and $\zeta(4,1)=\zeta(3,1,1)$. I also proved the "derivation theorem" that says, for any sequence of positive integers $(i_1,i_2,\dots,i_k)$ with $i_1>1$,

$$\sum_{j=1}^{k}\zeta(i_1,\dots,i_{j-1},i_j+1,i_{j+1},\dots,i_k)=\sum_{j=1}^{k}\sum_{p=0}^{l_j-2}\zeta(i_1,\dots,i_{j-1},i_j-p,p+1,i_{j+1},\dots,i_k)\tag{5}$$

where the empty sum is treated as zero. (For a proof see the section that follows.) Applying this to $(3,1)$ gives

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

and so $\zeta(3,2)=\zeta(2,2,1)$. Apply equation (5) to the sequence $(2,2)$ to get

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

so that $\zeta(2,3)=\zeta(2,1,2)$. Hence the third row in the diagram (4) is term-for-term identical to the second, and all the rows add up to $\zeta(5)$.

In weight 6 there are sixteen MZVs, which we arrange as follows.

$$\begin{aligned}&\zeta(6)\\&\zeta(5,1),\ \zeta(4,2),\ \zeta(3,3),\ \zeta(2,4)\\&\zeta(4,1,1),\ \zeta(3,2,1),\ \zeta(3,1,2),\ \zeta(2,3,1),\ \zeta(2,1,3),\zeta(2,2,2)\\&\zeta(3,1,1,1),\ \zeta(2,2,1,1),\ \zeta(2,1,2,1),\ \zeta(2,1,1,2)\\&\zeta(2,1,1,1,1)\end{aligned}\tag{6}$$

From equation (3) we match up entries in the first column: $\zeta(6)=\zeta(2,1,1,1,1)$, $\zeta(5,1)=\zeta(3,1,1,1)$. The sum of the second row is $\zeta(6)$, and the derivation theorem (5) applied to $(2,1,1,1)$ says that the sum of the sum of the fourth row is $\zeta(2,1,1,1,1)=\zeta(6)$. Now apply the derivation theorem to $(4,1)$, $(3,2)$, and $(2,3)$ to get

$$\zeta(5,1)+\zeta(4,2)=\zeta(4,1,1)+\zeta(3,2,1)+\zeta(2,3,1)\tag{7}$$

$$\zeta(4,2)+\zeta(3,3)=\zeta(3,1,2)+\zeta(2,2,2)+\zeta(3,2,1)\tag{8}$$

$$\zeta(3,3)+\zeta(2,4)=\zeta(2,1,3)+\zeta(2,3,1)+\zeta(2,2,2)\tag{9}$$

and similarly apply it to $(3,1,1)$, $(2,2,1)$, and $(2,1,2)$ to get

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

$$\zeta(3,2,1)+\zeta(2,3,1)+\zeta(2,2,2)=\zeta(2,1,2,1)+\zeta(2,2,1,1)\tag{11}$$

$$\zeta(3,1,2)+\zeta(2,2,2)+\zeta(2,1,3)=\zeta(2,1,1,2)+\zeta(2,1,2,1).\tag{12}$$

Add equations (7) and (9) to get

$$\zeta(6) = \zeta(4,1,1) + \zeta(3,2,1) + 2\zeta(2,3,1) + \zeta(2,1,3) + \zeta(2,2,2). \tag{13}$$

Similarly, we can add equations (10) and (12) to obtain

$$\zeta(4,1,1) + \zeta(3,2,1) + 2\zeta(3,1,2) + \zeta(2,2,2) + \zeta(2,1,3) = \zeta(6) \tag{14}$$

Comparing (13) and (14) gives

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

Using this fact, equation (13) says that the middle row of (6) adds to $\zeta(6)$. We can also compare equations (7) and (10) to get

$$\zeta(5,1) + \zeta(4,2) = \zeta(3,1,1,1) + \zeta(2,2,1,1),$$

or $\zeta(4,2) = \zeta(2,2,1,1)$.

Exercise 4. Conclude similarly that $\zeta(3,3) = \zeta(2,1,2,1)$ by comparing equations (8) and (11), and that $\zeta(2,4) = \zeta(2,1,1,2)$ by comparing equations (9) and (12).

The term-by-term equalities among the lines of (6) made me think about the correct generalization of (3). Here is one way to write it. Given a sequence $I = (i_1, \ldots, i_k)$ with $i_1 > 1$, let $\Sigma(I)$ be the sequence of partial sums, i.e.,

$$\Sigma(I) = (i_1, i_1 + i_2, \ldots, i_1 + \cdots + i_k).$$

Then $\Sigma(I)$ is a strictly increasing sequece of positive integers. Now let $\mathcal{I}_n$ be the set of (finite) strictly increasing sequences of positive integers whose last term is at most n, and define functions R_n and C_n on $\mathcal{I}_n$ by

$$R_n(a_1, \ldots, a_k) = (n+1-a_k, \ldots, n+1-a_1)$$
$$C_n(a_1, \ldots, a_k) = \text{complement in } \{1, \ldots, n\} \text{ of } \{a_1, \ldots, a_k\} \text{ arranged in increasing order}$$

Exercise 5. Show that $R_n^2 = \mathrm{id} = C_n^2$, and that $R_n C_n = C_n R_n$.

Then we can define an operation τ on sequences whose sum is n by

$$\tau(I) = \Sigma^{-1} R_n C_n \Sigma(I).$$

For example,

$$\tau(3,1,2) = \Sigma^{-1} R_6 C_6 (3,4,6) = \Sigma^{-1} R_6 (1,2,5) = \Sigma^{-1}(2,5,6) = (2,3,1).$$

Exercise 6. Check that $\tau(p+1, \underbrace{1, \ldots, 1}_{q-1}) = (q+1, \underbrace{1, \ldots, 1}_{p-1})$

I made the "duality conjecture" that $\zeta(I) = \zeta(\tau(I))$. The proof turns out to be almost embarassing simple, but requires another representation of $\zeta(I)$.

Exercise 7. For sequences I, J, let IJ be their juxtaposition (so if $I = (2,1,1)$ and $J = (3,2)$, then $IJ = (2,1,1,3,2)$). Show that $\tau(IJ) = \tau(J)\tau(I)$.

3. Proof of the derivation theorem

We first note that the definition of MZVs can be written

$$\zeta(i_1, \ldots, i_k) = \sum_{n_1, \ldots, n_k \geq 1} \frac{1}{s_k^{i_1} s_{n-1}^{i_2} \cdots s_1^{i_k}},$$

where $s_j = n_1 + \cdots + n_j$. Then evidently

$$\sum_{n_1,\ldots,n_k\geq 1} \frac{1}{s_k^{i_1}\cdots s_1^{i_k}} \sum_{j=1}^{s_k} \frac{1}{j} = \tag{15}$$
$$\zeta(i_1+1, i_2, \ldots, i_k) + \zeta(i_1, 1, i_2, \ldots, i_k) + \zeta(i_1, i_2+1, i_3, \ldots, i_k)$$
$$+ \cdots + \zeta(i_1, \ldots, i_{k-1}, i_k+1) + \zeta(i_1, \ldots, i_k, 1).$$

But the left-hand side of equation (15) can be written

$$\sum_{n_1,\ldots,n_k\geq 1} \frac{1}{s_1^{i_k} s_2^{i_{k-1}} \cdots s_k^{i_1}} \sum_{n_{k+1}=1}^{\infty} \left(\frac{1}{n_{k+1}} - \frac{1}{s_{k+1}}\right), \tag{16}$$

and by partial fractions we have

$$\frac{1}{n_{k+1}s_{k+1}^{i_1}} = \frac{1}{n_{k+1}s_k^{i_1}} - \sum_{j=0}^{i_1-1} \frac{1}{s_k^{j+1}s_{k+1}^{i_1-j}}$$

or

$$\frac{1}{s_k^{i_1}}\left(\frac{1}{n_{k+1}} - \frac{1}{s_{k+1}}\right) = \frac{1}{n_{k+1}s_{k+1}^{i_1}} + \sum_{j=0}^{i_1-2} \frac{1}{s_k^{j+1}s_{k+1}^{i_1-j}}.$$

Hence (16) is

$$\sum_{n_1,\ldots,n_{k+1}\geq 1} \frac{1}{s_1^{i_k}\cdots s_{k-1}^{i_2} n_{k+1} s_{k+1}^{i_1}} + \sum_{j=0}^{i_1-2} \sum_{n_1,\ldots,n_{k+1}\geq 1} \frac{1}{s_1^{i_1}\cdots s_{k-1}^{i_2} s_k^{j+1} s_{k+1}^{i_1-j}}$$

or, since the first sum is unchanged by permuting n_k and n_{k+1},

$$\sum_{n_1,\ldots,n_{k+1}\geq 1} \frac{1}{s_1^{i_k}\cdots s_{k-1}^{i_2} n_k s_{k+1}^{i_1}} + \sum_{j=0}^{i_1-2} \zeta(i_1-j, j+1, \ldots, i_2, \ldots, i_k).$$

Now use the partial-fractions expansion

$$\frac{1}{n_k s_k^{i_2}} = \frac{1}{n_k s_{k-1}^{i_2}} - \sum_{j=0}^{i_2-1} \frac{1}{s_{k-1}^{j+1}s_k^{i_2-j}}$$

to write the first sum as

$$\sum_{n_1,\ldots,n_{k+1}\geq 1} \frac{1}{s_1^{i_k}\cdots s_{k-2}^{i_3} n_{k-1} s_k^{i_2} s_{k+1}^{i_1}} + \sum_{j=0}^{i_2-1} \zeta(i_1, i_2-j, j+1, i_3, \ldots, i_k).$$

Continue in this way to write (16) as

$$\sum_{p=1}^{k}\sum_{j=0}^{i_p-2} \zeta(i_1, \ldots, i_{p-1}, i_p-j, j+1, i_{p+1}, \ldots, i_k) + \sum_{n_1,\ldots,n_{k+1}\geq 1} \frac{1}{n_1 s_2^{i_k}\cdots s_{k+1}^{i_1}},$$

with the last sum evidently equal to $\zeta(i_1, \ldots, i_k, 1)$. Now replace the left-hand side of equation (15) with this expression, and after cancellation equation (5) follows.

Historical note. The first publications to consider multiple zeta values of arbitrary depth were my paper [**7**] and that by Don Zagier [**17**]. The sum conjecture was proved by Andrew Granville [**6**] and Zagier (unpublished).

CHAPTER 2

The Depth Two Case

1. Tornheim sums

The following sums were introduced by Tornheim [**15**]:

$$T(p,q;r)=\sum_{k_1,k_2\ge 1}\frac{1}{k_1^p k_2^q (k_1+k_2)^r}.$$

Such a sum converges if $p+r, q+r$, and $p+q+r$ are all ≥ 2. Clearly $T(p,q;r)=T(q,p;r)$, and $T(p,0,r)=\zeta(r,p)$. The key facts about these sums are the following: first,

$$T(p,q;r)=T(p-1,q;r+1)+T(p,q-1;r+1). \tag{17}$$

whenever both side converge; second,

$$T(1,q;1)=\sum_{k_1,k_2\ge 1}\frac{1}{k_1 k_2^q (k_1+k_2)}=\zeta(q+2)+\zeta(q+1,1) \tag{18}$$

for $q\ge 1$; and third,

$$T(p,q;0)=\zeta(p)\zeta(q)=\zeta(p+q)+\zeta(p,q)+\zeta(q,p). \tag{19}$$

if $p,q\ge 2$.

Exercise 8. Prove equations (17), (18), and (19). Hint for (18): note that

$$\sum_{k_1=1}^{\infty}\frac{1}{k_1(k_1+k_2)}=\sum_{k_1=1}^{\infty}\left[\frac{1}{k_1k_2}-\frac{1}{k_2(k_1+k_2)}\right]=\frac{1}{k_2}\sum_{j=1}^{k_2}\frac{1}{j}.$$

For multiple zeta values of depth two, we have the following set of identities involving binomial coefficients.

THEOREM 1. *For integer $1\le p\le q$ with $p+q=n\ge 3$,*

$$\zeta(n)=\sum_{i=p+1}^{n-1}\binom{i-1}{p-1}\zeta(i,n-i)+\sum_{i=q+1}^{n-1}\binom{i-1}{q-1}\zeta(i,n-i), \tag{20}$$

where empty sums are interpreted as zero.

PROOF. The theorem is then a consequence of the following result: if $p,q\ge 2$ and $r\ge 0$, or if $p,q\ge 1$ and $r\ge 1$, then

$$T(p,q;r)=\sum_{i=p}^{p+q-1}\binom{i-1}{p-1}\zeta(r+i,p+q-i)+\sum_{i=q}^{p+q-1}\binom{i-1}{q-1}\zeta(r+i,p+q-i). \tag{21}$$

To obtain equation (20) in case $p\ge 2$, set $r=0$ in equation (21) and then use equation (19). If $p=1$, set $r=1$ in equation (21) and use equation (18).

We prove equation (21) by induction on $p+q$. To start the induction we must prove (21) for $p=q=2$, $r\geq 0$, and for $q=1$, $r\geq 1$. In the first case we have

$$\begin{aligned}T(2,2;r)&=T(1,2;r+1)+T(2,1;r+1)\\&=T(0,2;r+2)+2T(1,1;r+2)+T(2,0;r+2)\\&=2T(2,0;r+2)+4T(1,0;r+3)\\&=2\sum_{i=2}^{3}\binom{i-1}{1}\zeta(r+i,4-i)\end{aligned}$$

In the second we have

$$\begin{aligned}T(p,1;r)&=T(p,0;r+1)+T(p-1,1;r+1)\\&=\zeta(r+1,p)+\zeta(r+2,p-1)+T(p-2,1;r+2)\\&=\cdots\\&=\sum_{i=p}^{p}\binom{i-1}{p-1}\zeta(r+i,p+1-i)+\sum_{i=1}^{p}\binom{i-1}{0}\zeta(r+i,p+1-i).\end{aligned}$$

Finally, if $p+q=n$, $p,q\geq 2$, and equation (21) holds for smaller values of p,q, then

$$\begin{aligned}T(p,q;r)&=T(p-1,q;r+1)+T(p,q-1;r+1)\\&=\sum_{i=p-1}^{n-2}\binom{i-1}{p-2}\zeta(r+i+1,n-1-i)+\sum_{i=q}^{n-2}\binom{i-1}{q-1}\zeta(r+i+1,n-1-i)\\&\quad+\sum_{i=p}^{n-2}\binom{i-1}{p-1}\zeta(r+i+1,n-1-i)+\sum_{i=q-1}^{n-2}\binom{i-1}{q-2}\zeta(r+i+1,n-1-i)\\&=\sum_{i=p-1}^{n-2}\binom{i}{p-1}\zeta(r+i+1,n-1-i)+\sum_{i=q-1}^{n-2}\binom{i}{q-1}\zeta(r+i+1,n-1-i)\\&=\sum_{i=p}^{n-1}\binom{i-1}{p-1}\zeta(r+i,n-i)+\sum_{i=q}^{n-1}\binom{i-1}{q-1}\zeta(r+i,n-i).\end{aligned}$$

□

If in the preceding result we set $p=1$, $q=n-1$, it reads

$$\zeta(n)=\sum_{i=2}^{n-1}\zeta(i,n-i),\tag{22}$$

which is just the sum theorem for depth 2. But of course these relations give us more: let's look at the case $n=5$. Besides the sum theorem for depth 2 ($p=1$), for $p=2$ we have

$$\zeta(5)=\sum_{i=3}^{4}\binom{i-1}{1}\zeta(i,5-i)+\binom{3}{2}\zeta(4,1)=6\zeta(4,1)+2\zeta(3,2).\tag{23}$$

Subtract this from $\zeta(5)=\zeta(4,1)+\zeta(3,2)+\zeta(2,3)$ to get

$$\zeta(4,1)=\frac{1}{5}\zeta(2,3)-\frac{1}{5}\zeta(3,2).$$

It then follows that

$$\zeta(5) = \frac{4}{5}\zeta(3,2) + \frac{6}{5}\zeta(2,3),$$

so all the MZVs of weight 5 are rational linear combinations of $\zeta(2,3)$ and $\zeta(3,2)$.

Exercise 9. Work out the relations from Theorem 1 for weight 6.

Exercise 10. Multiply both sides of $\zeta(2,2) = \frac{3}{4}\zeta(4)$ by $\zeta(2)$ to show that $\frac{3}{16}\zeta(6) = \zeta(2,2,2)$.

Since $\zeta(6) = \frac{\pi^6}{945}$, it follows from the preceding exercise that

$$\zeta(2,2,2) = \frac{\pi^6}{5040}.$$

In fact, as shown in [**7**], there is a general result

$$\zeta(\underbrace{2,\ldots,2}_{n}) = \frac{\pi^{2n}}{(2n+1)!}. \tag{24}$$

This can be expressed in terms of so-called generating functions as

$$\sum_{n=0}^{\infty} \zeta(\underbrace{2,\ldots,2}_{n})x^{2n} = \frac{\sin \pi x}{\pi x}.$$

In [**1**] further results of this kind are obtained, including

$$\zeta(\underbrace{4,\ldots,4}_{n}) = \frac{2^{2n+1}\pi^{4n}}{(4n+2)!} \quad \text{and} \quad \zeta(\underbrace{6,\ldots,6}_{n}) = \frac{6(2\pi)^{6n}}{(6n+3)!}.$$

Exercise 11. Using the previous two exercises and the results of the previous lecture, show that all MZVs of weight 6 can be written as rational linear combinations of $\zeta(3,3)$ and $\zeta(2,2,2)$.

In fact, all MZVs of weight n are rational linear combinations of the weight n MZVs corresponding to sequences that only have 2's and 3's. I conjectured this in [**8**], and it was proved recently by Francis Brown [**3**] with an essential contribution from Don Zagier [**18**].

Exercise 12. (For those with some background in combinatorics) Prove that the number of sequences of weight n that involve only 2's and 3's is the nth Padovan number P_n, where $P_1 = 0$, $P_2 = 1$, $P_3 = 1$, and $P_n = P_{n-2} + P_{n-3}$ for $n \geq 4$.

2. Weighted sum formulas

Gangl, Kaneko and Zagier [**5**] rewrote Theorem 1 in a clever way. First define, for $n \geq 3$,

$$\mathfrak{Z}_n(x,y) = \sum_{j=2}^{n-1} x^{j-1}y^{n-j-1}\zeta(j, n-j).$$

Then Theorem 1 can be expressed as

$$\mathfrak{Z}_n(x+y,x) + \mathfrak{Z}_n(x+y,y) = \mathfrak{Z}_n(x,y) + \mathfrak{Z}_n(y,x) + (x^{n-2} + x^{n-3}y + \cdots + xy^{n-3} + y^{n-2})\zeta(n), \tag{25}$$

as can be seen by checking the coefficient of each monomial $x^{p-1}y^{q-1}$, for $p+q=n$.

Exercise 13. Do this.

The advantage of equation (25) is that it makes it easy to prove various "weighted sum formulas," i.e., formulas of the type

$$\sum_{j=2}^{n-1} a_j \zeta(j, n-j) = f(n)\zeta(n).$$

Euler's sum theorem is just the case where $a_j = 1$ for all j and $f(n) = 1$. This follows upon setting $y = 0$ in equation (25). The following result was obtained by Ohno and Zudilin [**11**].

Corollary 1. *For $n \geq 3$,*

$$\sum_{i=2}^{n-1} 2^i \zeta(i, n-i) = (n+1)\zeta(n).$$

Proof. Set $x = y = 1$ in equation (25), and use equation (22). □

If $n = 2m$ is even, we have the following, which was obtained by Euler [**4**].

Corollary 2. *For $m \geq 1$,*

$$\sum_{i=1}^{2m-2} (-1)^i \zeta(2m-i, i) = \frac{1}{2}\zeta(2m).$$

Proof. Set $x = 1$, $y = -1$ in equation (25). □

Notice that it follows from the preceding corollary and the sum theorem that

$$\sum_{i=1}^{m-1} \zeta(2i, 2m-2i) = \frac{3}{4}\zeta(2m)$$

and

$$\sum_{i=2}^{m} \zeta(2i-1, 2m-2i+1) = \frac{1}{4}\zeta(2m),$$

though this seems not to have been noticed in print before [**5**].

For n odd, there are the following results. The first appears in Euler's paper [**4**].

Corollary 3. *If $n = 2m+1$, then*

$$2\zeta(2, n-2) + \sum_{j=2}^{2m} (-1)^j (n-2j)\zeta(j, n-j) = m\zeta(n).$$

Proof. Differentiate both sides of equation (25) with respect to x, and then set $(x, y) = (1, -1)$. □

Corollary 4. *If $n = 4m+1$, then*

$$\sum_{j=2}^{4m} \left[2^{\frac{j}{2}} \cos\frac{j\pi}{4} - 2^{\frac{1}{2}} \sin\left(\frac{j\pi}{2} + \frac{\pi}{4}\right) \right] \zeta(j, n-j) = 0.$$

If $n = 4m+3$, then

$$\sum_{j=2}^{4m+2} \left[2^{\frac{j}{2}} \sin\frac{j\pi}{4} + 2^{\frac{1}{2}} \cos\left(\frac{j\pi}{2} + \frac{\pi}{4}\right) \right] \zeta(j, n-j) = \zeta(n).$$

PROOF. Set $(x, y) = (1, i)$ in equation (25) and simplify. □

Exercise 14. Carry out the details of the last proof.

3. Which double zeta values are reducible?

It is natural to ask which double zeta values $\zeta(m, n)$ can be expressed (as polynomials with rational coefficients) in terms of the single zeta values $\zeta(i)$. Call such a double zeta value "reducible". It is easy to see that $\zeta(n-1, 1)$ is always reducible, using equation (22) together with

$$\zeta(i, n-i) = \zeta(i)\zeta(n-i) - \zeta(n)$$

for all $2 \le i \le n-2$. The result is

$$\zeta(n-1, 1) = \frac{n-1}{2}\zeta(n) - \frac{1}{2}\sum_{i=2}^{n-2}\zeta(i)\zeta(n-i),$$

which was given by Euler. In fact, all double zeta values (and indeed all multiple zeta values) through weight 7 are reducible, but this seems to hit a brick wall at weight 8: no one has been able to write $\zeta(2, 6)$ as a rational polynomial in the single zeta values. Nevertheless, it is possible to reduce $\zeta(m, n)$ in the case where $m + n = 2k + 1$ is odd, and indeed formulas can be extracted from Euler's paper [**4**]. If m is even and n is odd,

$$\begin{aligned}\zeta(m, n) = \frac{1}{2}\left[\binom{m+n}{m} - 1\right]\zeta(m+n) + \zeta(m)\zeta(n) \\ - \sum_{j=1}^{k}\left[\binom{2j-2}{m-1} + \binom{2j-2}{n-1}\right]\zeta(2j-1)\zeta(m+n-2j+1),\end{aligned}$$

while if m is odd and n is even,

$$\begin{aligned}\zeta(m, n) = -\frac{1}{2}\left[\binom{m+n}{m} + 1\right]\zeta(m+n) \\ + \sum_{j=1}^{k}\left[\binom{2j-2}{m-1} + \binom{2j-2}{n-1}\right]\zeta(2j-1)\zeta(m+n-2j+1).\end{aligned}$$

The generalization (due to Zagier and Tsumura idependently) is that a MZV can be reduced to lower depth if its depth and weight have opposite parity.

CHAPTER 3

The Algebraic Approach

1. Iterated integral representation

Besides the series representation (2), MZVs can be written as iterated integrals. For example,

$$\int_0^1 \frac{dt_2}{t_2}\int_0^{t_2}\frac{dt_1}{1-t_1} = \int_0^1 \frac{dt_2}{t_2}\int_0^{t_2}\sum_{j=1}^{\infty} t_1^{j-1}dt_1 = \int_0^1 \frac{dt_2}{t_2}\sum_{j=1}^{\infty}\frac{t_2^j}{j} = \sum_{j=1}^{\infty}\int_0^1 \frac{t_2^{j-1}}{j}dt_2 = \sum_{j=1}^{\infty}\frac{1}{j^2} = \zeta(2). \tag{26}$$

By making the associations

$$x \leftrightarrow \frac{dt}{t} \quad \text{and} \quad y \leftrightarrow \frac{dt}{1-t}$$

we can encode such integral representations algebraically: for example, the left-hand side of equation (26) is encoded as xy. The iterated integral corresponding to $x^{n-1}y$, that is,

$$\int_0^1 \frac{dt_n}{t_n}\int_0^{t_n}\frac{dt_{n-1}}{t_{n-1}}\cdots\int_0^{t_3}\frac{dt_2}{t_2}\int_0^{t_2}\frac{dt_1}{1-t_1},$$

gives $\zeta(n)$ for $n \geq 2$.

Exercise 15. Prove this.

Now suppose we have $x^{m-1}yx^{n-1}y$, or

$$\int_0^1 \frac{dt_{n+m}}{t_{n+m}}\cdots\int_0^{t_{n+3}}\frac{dt_{n+2}}{t_{n+2}}\int_0^{t_{n+2}}\frac{dt_{n+1}}{1-t_{n+1}}\int_0^{t_{n+1}}\frac{dt_n}{t_n}\cdots\int_0^{t_3}\frac{dt_2}{t_2}\int_0^{t_2}\frac{dt_1}{1-t_1}.$$

This is evidently

$$\int_0^1 \frac{dt_{n+m}}{t_{n+m}}\cdots\int_0^{t_{n+3}}\frac{dt_{n+2}}{t_{n+2}}\int_0^{t_{n+2}}\frac{dt_{n+1}}{1-t_{n+1}}\sum_{j=1}^{\infty}\frac{t_{n+1}^j}{j^n} =$$

$$\int_0^1 \frac{dt_{n+m}}{t_{n+m}}\cdots\int_0^{t_{n+3}}\frac{dt_{n+2}}{t_{n+2}}\int_0^{t_{n+2}}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\frac{t_{n+1}^{i+j-1}}{j^n}dt_{n+1} =$$

$$\int_0^1 \frac{dt_{n+m}}{t_{n+m}}\cdots\int_0^{t_{n+3}}\sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\frac{t_{n+2}^{i+j-1}}{(i+j)j^n}dt_{n+2} = \sum_{i=1}^{\infty}\sum_{j=1}^{\infty}\frac{1}{(i+j)^m j^n} = \zeta(m,n).$$

More generally, the iterated integral $x^{i_1-1}yx^{i_2-1}y\cdots x^{i_k-1}y$ represents $\zeta(i_1,\dots,i_k)$ (and converges exactly when $i_1 > 1$).

We shall use monomials in noncommuting variables x and y to represent MZVs: we denote the ring of such monomials (with rational coefficients) by $\mathbb{Q}\langle x,y\rangle$. Note that $\mathbb{Q}\langle x, y\rangle$ includes an identity element 1 as the empty monomial. We write $\mathfrak{H}$ if we just want to think about the rational vector space structure of $\mathbb{Q}\langle x, y\rangle$ and not its (noncommutative) product. For our monomials to represent convergent MZVs, they must always begin with x and end with y: the rational vector space generated by such monomials (and 1) is denoted $\mathfrak{H}^0$. We note that $\mathfrak{H}^0$ is a subalgebra: that is, $ab \in \mathfrak{H}^0$ if a, b are in $\mathfrak{H}^0$. The degree $|w|$ of a monomial w of $\mathfrak{H}$ is simply the total number of x's and y's in w. We define the depth $d(w)$ of a monomial w to be the total number of y's appearing in w. In this notation, the sum and duality theorems mentioned in Lecture 1 can be stated as follows. The sum theorem is

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

for $n \geq 2$. For the duality theorem, define an antiautomorphism τ of the noncommutative polynomial ring $\mathbb{Q}\langle x, y\rangle$ in x and y by $\tau(x) = y$. $\tau(y) = x$; note that $\tau^2 = \mathrm{id}$ and tau preserves degree.

Exercise 16. Show that if I is associated to the monomial w, then $\tau(I)$ (as defined in Lecture 1) is associated to $\tau(w)$.

Then the duality theorem becomes both very easy to state and to prove.

Theorem 2. *For monomials $w \in \mathfrak{H}^0$, $\zeta(w) = \zeta(\tau(w))$.*

Proof. Make the change of variable

$$(t_1, \ldots, t_n) \to (1 - t_n, \ldots, 1 - t_1)$$

and observe that it transforms the iterated integral corresponding to w into that corresponding to $\tau(w)$. ☐

Another important fact about iterated integrals is how they multiply. For example,

$$\begin{aligned}\int_0^1 f(x)dx \cdot \int_0^1 g(y)dy &= \iint_{0\leq y\leq x\leq 1} f(x)g(y)dxdy + \iint_{0\leq x\leq y\leq 1} f(x)g(y)dxdy \\ &= \int_0^1 f(x)dx \int_0^x g(y)dy + \int_0^1 g(y)dy \int_0^y f(x)dx.\end{aligned}$$

More generally, this type of multiplication is called "shuffle product." Thought of on monomials, is consists of all the ways of "shuffling" them together. For example the shuffle product of xy (associated with $\zeta(2)$) and x^2y (associated with $\zeta(3)$) is

$$xyx^2y + x^2yxy + 2x^3y^2 + x^2yxy + 2x^3y^2 + 2x^3y^2 + x^2yxy = xyx^2y + 3x^2yxy + 6x^3y^2$$

which is associated with $\zeta(2, 3) + 3\zeta(3, 2) + 6\zeta(4, 1)$. So evidently

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

which is very different from the series multiplication

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

Exercise 17. Compare these two equations and deduce equation (23) from the last lecture.

If we formulate the series multiplication (or "stuffle product") in terms of the algebraic notation, we get the "harmonic algebra" of [**8**].

Another big advantage of this notation is that it makes the derivation theorem of Lecture 1 much simpler to state. A derivation is just a linear function D from an algebra to itself with the property that

$$D(ab) = D(a)b + aD(b).$$

Exercise 18. Show that if the algebra has an identity element (that is, an element 1 so that $1x = x1 = x$ for every x in the algebra), then any derivation takes 1 to 0.

Let D be the derivation of $\mathbb{Q}\langle x, y\rangle$ with $D(x) = 0$ and $D(y) = xy$. Then D takes $\mathfrak{H}^0$ to itself, as does the derivation $\tau D\tau$. We can state the derivation theorem as

$$\zeta(D(w)) = \zeta(D(\tau(w))) \tag{27}$$

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

Exercise 19. Check that if I is associated with the monomial w, then equation (27) coincides with the derivation theorem (5) for I.

The proof of the derivation theorem in [**7**] is an elementary but messy partial-fractions argument. (For a deeper but more transparent argument, see Exercise 23 below.) The derivation theorem seems to have nothing to do with iterated integrals, but the algebraic notation is working some magic here–just compare equation (27) with equation (5) in Lecture 1.

2. The shuffle algebra

As above, let $\mathfrak{H}$ be the underlying graded rational vector space of $\mathbb{Q}\langle x, y\rangle$, with x and y both given degree 1. We 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 monomial w, $1 \sqcup\!\sqcup w = w \sqcup\!\sqcup 1 = w$;
S2. For any monomial w_1, w_2 and $a, b \in \{x, y\}$,

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

We have the following result.

THEOREM 3. *The $\sqcup\!\sqcup$-product is commutative and associative.*

PROOF. The idea is to use induction on degree. First let's consider commutativity. It's enough to show that $u \sqcup\!\sqcup w - w \sqcup\!\sqcup u = 0$ for any monomials u, w. We induct on $|u| + |w|$. The result is obvious for $|u| + |w| = 0$ (since in that case $u = w = 1$). Suppose monomials whose degrees sum to $< n$ commute, and let $|u| + |w| = n$. Let $u = au'$ and $w = bw'$ for $a, b \in \{x, y\}$. Then

$$\begin{aligned} u \sqcup\!\sqcup w - w \sqcup\!\sqcup u &= a(u' \sqcup\!\sqcup w) + b(u \sqcup\!\sqcup w') - b(w' \sqcup\!\sqcup u) - a(w \sqcup\!\sqcup u') \\ &= a(u' \sqcup\!\sqcup w - w \sqcup\!\sqcup u') + b(u \sqcup\!\sqcup w' - w' \sqcup\!\sqcup u) = 0, \end{aligned}$$

since $u' \sqcup\!\sqcup w - w \sqcup\!\sqcup u' = 0 = u \sqcup\!\sqcup w' - w' \sqcup\!\sqcup u$ by the induction hypothesis.

For associativity, it is enough to show that

$$(u \sqcup\!\sqcup v) \sqcup\!\sqcup w - u \sqcup\!\sqcup (v \sqcup\!\sqcup w) = 0$$

for all monomials u, v, w. We use induction on $|u|+|v|+|w|$. The result is immediate for $|u| + |v| + |w| = 0$, so suppose it holds for $|u| + |v| + |w| < n$ and let u, v, w be monomials whose degrees sum to n. Write $u = au'$, $v = bv'$, and $w = cw'$. Then

$$\begin{aligned}
(u \sqcup\!\sqcup v) \sqcup\!\sqcup w - u \sqcup\!\sqcup (v \sqcup\!\sqcup w) &= (au' \sqcup\!\sqcup bv') \sqcup\!\sqcup cw' - au' \sqcup\!\sqcup (bv' \sqcup\!\sqcup cw') \\
&= (a(u' \sqcup\!\sqcup v) + b(u \sqcup\!\sqcup v')) \sqcup\!\sqcup cw' - au' \sqcup\!\sqcup (b(v' \sqcup\!\sqcup w) + c(v \sqcup\!\sqcup w')) \\
&= a((u' \sqcup\!\sqcup v) \sqcup\!\sqcup w) + c(a(u' \sqcup\!\sqcup v) \sqcup\!\sqcup w') + b((u \sqcup\!\sqcup v') \sqcup\!\sqcup w) + c(b(u \sqcup\!\sqcup v') \sqcup\!\sqcup w') \\
&\quad - a(u' \sqcup\!\sqcup (b(v' \sqcup\!\sqcup w))) - b(u \sqcup\!\sqcup (v' \sqcup\!\sqcup w)) - a(u' \sqcup\!\sqcup (c(v \sqcup\!\sqcup w'))) - c(u \sqcup\!\sqcup (v \sqcup\!\sqcup w')) \\
&= a((u' \sqcup\!\sqcup v) \sqcup\!\sqcup w - u' \sqcup\!\sqcup (b(v' \sqcup\!\sqcup w)) - u' \sqcup\!\sqcup (c(v \sqcup\!\sqcup w'))) + b((u \sqcup\!\sqcup v') \sqcup\!\sqcup w - u \sqcup\!\sqcup (v' \sqcup\!\sqcup w)) \\
&\quad + c(a(u' \sqcup\!\sqcup v) \sqcup\!\sqcup w' + b(u \sqcup\!\sqcup v') \sqcup\!\sqcup w' - u \sqcup\!\sqcup (v \sqcup\!\sqcup w')) \\
&= a((u' \sqcup\!\sqcup v) \sqcup\!\sqcup w - u' \sqcup\!\sqcup (v \sqcup\!\sqcup w)) + b(0) + c((u \sqcup\!\sqcup v) \sqcup\!\sqcup w' - u \sqcup\!\sqcup (v \sqcup\!\sqcup w')) = 0
\end{aligned}$$

where we have used the induction hypothesis. $\square$

So $\mathfrak{H}$ with the multiplication $\sqcup\!\sqcup$ is a commutative algebra on the noncommuative monomials. (This might seem weird at first, but one gets used to it.) When we want to refer to the ring with additive group $\mathfrak{H}$ and $\sqcup\!\sqcup$ as multiplication, we write $(\mathfrak{H}, \sqcup\!\sqcup)$. Recall from the previous section that τ is the anti-automorphism of $\mathbb{Q}\langle x, y\rangle$ the exchanges x and y. It needn't be true that τ is a homomorphism for the $\sqcup\!\sqcup$ product, but it turns out to be.

Theorem 4. *τ is an automorphism of $(\mathfrak{H}, \sqcup\!\sqcup)$.*

Proof. Since evidently $\tau^2 = \mathrm{id}$, it suffices to show that τ is a $\sqcup\!\sqcup$-homomorphism. Using the axioms S1, S2 above and induction on $|w_1 w_2|$, it is straightforward to prove that

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

for any monomials w_1, w_2 and $a, b \in \{x, y\}$. Now suppose inductively that $\tau(w_1 \sqcup\!\sqcup w_2) = \tau(w_1) \sqcup\!\sqcup \tau(w_2)$ for $|w_1 w_2| < n$, and let w_1, w_2 be monomials with $|w_1 w_2| = n$. We can assume both w_1 and w_2 are nonempty; write $w_1 = w_1' a$ and $w_2 = w_2' b$. Then

$$\begin{aligned}
\tau(w_1 \sqcup\!\sqcup w_2) &= \tau((w_1' \sqcup\!\sqcup w_2)a + (w_1 \sqcup\!\sqcup w_2')b) \\
&= \tau(a)\tau(w_1' \sqcup\!\sqcup w_2) + \tau(b)\tau(w_1 \sqcup\!\sqcup w_2') \\
&= \tau(a)(\tau(w_1') \sqcup\!\sqcup \tau(w_2)) + \tau(b)(\tau(w_1) \sqcup\!\sqcup \tau(w_2')) \\
&= \tau(a)\tau(w_1') \sqcup\!\sqcup \tau(b)\tau(w_2') \\
&= \tau(w_1) \sqcup\!\sqcup \tau(w_2).
\end{aligned}$$

$\square$

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

Exercise 20. Find all the Lyndon monomials of weight 5.

From [**12**] we have the following result.

Theorem 5. *The commutative algebra $(\mathfrak{H}, \sqcup\!\sqcup)$ is a polynomial algebra on the Lyndon monomials.*

The link between the shuffle algebra and MZVs is given by the iterated integral representation, together with the fact that iterated integrals multiply by shuffle product. We can state this as follows.

THEOREM 6. *The map $\zeta : (\mathfrak{H}^0, ш) \to \mathbb{R}$ is a τ-equivariant homomorphism.*

The shuffle-product structure has been used to prove some MZV identities. For example, in [**2**] it is first established that

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

in $\mathfrak{H}$, and then ζ is applied 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 (24), which in the algebraic notation is

$$\zeta((xy)^k) = \frac{\pi^{2k}}{(2k+1)!}, \tag{28}$$

one obtains from this the result conjectured by Zagier [**17**] several years earlier:

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

In terms of the sequence notation, this is

$$\zeta(\underbrace{3,1,3,1,\dots,3,1}_{n \text{ blocks}}) = \frac{1}{2n+1}\zeta(\underbrace{2,\dots,2}_{2n}) = \frac{2\pi^{4n}}{(4n+2)!}.$$

3. The harmonic algebra

We can define another commutative multiplication $*$ on $\mathfrak{H}$ by requiring that it distribute over the addition and that it satisfy the following axioms:

H1. For any monomial w, $1 * w = w * 1 = w$;

H2. For any monomial w and integer $n \geq 1$,

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

H3. For any monomials w_1, w_2 and integers $p, q \geq 0$,

$$x^p y w_1 * x^q y w_2 = x^p y(w_1 * x^q y w_2) + x^q y(x^p y w_1 * w_2) + x^{p+q+1} y(w_1 * w_2).$$

Note that axiom (H3) allows the $*$-product of any pair of monomials to be computed recursively, since each $*$-product on the right has fewer factors of y than the $*$-product on the left-hand side. We have the following counterpart of Theorem 3.

THEOREM 7. *The $*$-product is commutative and associative.*

Exercise 21. To prove this it's enough to show that

$$u * v - v * u = 0, \quad u * (v * w) - (u * v) * w = 0$$

for all monomials u, v, w of $\mathfrak{H}$. Use induction on depth.

We refer to $\mathfrak{H}$ together with its commutative multiplication $*$ as the harmonic algebra $(\mathfrak{H}, *)$.

Exercise 22. Show by example that τ is *not* a homomorphism of $(\mathfrak{H}, *)$.

We do have counterparts of Theorems 5 and 6, which are proved in [**8**].

THEOREM 8. *The commutative algebra $(\mathfrak{H}, *)$ is a polynomial algebra on the Lyndon monomials.*

THEOREM 9. $(\mathfrak{H}^0, *)$ *is a subalgebra of* $(\mathfrak{H}, *)$*, and* $\zeta : (\mathfrak{H}^0, *) \to \mathbb{R}$ *is a homomorphism.*

The axioms above may seem mysterious, but here is a simpler description. Let $\mathfrak{H}^1$ be the vector subspace $\mathbb{Q}1 + \mathfrak{H}y$ of $\mathfrak{H}$; it is evidently a subalgebra of $(\mathfrak{H}, *)$. In fact, since x is the only Lyndon monomial ending in x, it is easy to see that $\mathfrak{H}^1$ is the subalgebra of $(\mathfrak{H}, *)$ generated by the Lyndon monomials other than x. Note that any monomials $w \in \mathfrak{H}^1$ can be written in terms of the elements $z_i = x^{i-1}y$, and that the y-degree $d(w)$ is the number of factors in w when expressed this way. We can rewrite the inductive rule (H3) for the $*$-product as

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

Thus, for example,

$$\begin{aligned} z_2 z_1 * z_3 &= z_2(z_1 * z_3) + z_3(z_2 z_1 * 1) + z_5(z_1 * 1) = \\ &\quad z_2(z_1(1 * z_3) + z_3(z_1 * 1) + z_4(1 * 1)) + z_3 z_2 z_1 + z_5 z_1 = \\ &\qquad z_2 z_1 z_3 + z_2 z_3 z_1 + z_2 z_4 + z_3 z_2 z_1 + z_5 z_1, \end{aligned}$$

corresponding to the fact that

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

Because the multiplications $*$ and $\sqcup\!\sqcup$ are quite different, Theorems 6 and 9 imply that the kernel of ζ (that is, the subspace of $\mathfrak{H}^0$ that ζ sends to 0) is quite large. At the beginning of this lecture we computed

$$xy \sqcup\!\sqcup x^2 y = xyx^2y + 3x^2yxy + 6x^3y^2$$

and

$$xy * x^2y = xyx^2y + x^2yxy + x^4y$$

from which follow

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

In fact, it has been conjectured that all identities of MZVs come from comparing the two multiplications. One concrete example is the derivation theorem.

Exercise 23. Show that

$$y \sqcup\!\sqcup w - y * w = \tau D \tau(w) - D(w)$$

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

CHAPTER 4

Cyclic Derivations and the Sum Theorem

1. The cyclic derivation theorem

In my first paper on multiple zeta values I discovered and proved the derivation theorem, but this wasn't sufficient to prove the sum theorem. But a few years later I discovered an odd relative of the derivation theorem, which actually has the sum theorem as a corollary: I call it the cyclic derivation theorem. The proof was supplied by Yasuo Ohno, and appears in our joint paper [**9**]. The statement of this theorem in the sequence notation should be compared to the statement (5) of the derivation theorem in Lecture 1.

Theorem 10. *For any sequence $i_1, \ldots, i_k$ of positive integers with some $i_j \geq 2$,*

$$\sum_{j=1}^{k} \zeta(i_j + 1, i_{j+1}, \ldots, i_k, i_1, \ldots, i_{j-1}) =$$

$$\sum_{\{j \mid i_j \geq 2\}} \sum_{q=0}^{i_j - 2} \zeta(i_j - q, i_{j+1}, \ldots, i_k, i_1, \ldots, i_{j-1}, q+1).$$

To see why this is called the "cyclic" derivation theorem, let's apply it to the sequence $(2, 1, 3, 1)$. In this case the theorem says

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

This may be contrasted with the derivation theorem applied to the same sequence:

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

In the next section I will give Yasuo's proof of this result, and in the following one I will give an algebraic presentation of the theorem very close to (27).

2. An unenlightening (but elementary) proof

Here is a proof of Theorem 10 using partial fractions. For positive integers $i_1, \ldots, i_k$, and a nonnegative integer i_{k+1}, define

$$R(i_1, \ldots, i_k) = \sum_{n_1 > \cdots > n_k > n_{k+1} \geq 0} \frac{1}{(n_1 - n_{k+1}) n_1^{i_1} \cdots n_k^{i_k}}$$

and

$$S(i_1, \ldots, i_k, i_{k+1}) = \sum_{n_1 > \cdots > n_{k+1} > 0} \frac{1}{(n_1 - n_{k+1}) n_1^{i_1} \cdots n_{k+1}^{i_{k+1}}}.$$

It is immediate from these definitions that

$$S(i_1,\dots,i_k,0) = R(i_1,\dots,i_k) - \zeta(i_1+1,i_2,\dots,i_k). \tag{29}$$

Also, from

$$\frac{1}{n_1(n_1-n_{k+1})} = \frac{1}{n_{k+1}}\left(\frac{1}{n_1-n_{k+1}} - \frac{1}{n_1}\right)$$

it follows that

$$S(i_1,\dots,i_k,i_{k+1}) = S(i_1-1,i_2,\dots,i_k,i_{k+1}+1) - \zeta(i_1,\dots,i_k,i_{k+1}+1) \tag{30}$$

and that

$$\begin{aligned}\sum_{n_1>\cdots>n_{k+1}>0} \frac{1}{(n_1-n_{k+1})n_1 n_2^{i_2}\cdots n_{k+1}^{i_{k+1}}} &= \sum_{n_1>\cdots>n_{k+1}>0} \frac{1}{n_2^{i_2}\cdots n_k^{i_k} n_{k+1}^{i_{k+1}}}\left(\frac{1}{n_1-n_{k+1}} - \frac{1}{n_1}\right)\\
&= \sum_{n_2>\cdots>n_{k+1}>0} \frac{1}{n_2^{i_2}\cdots n_k^{i_k} n_{k+1}^{i_{k+1}}} \sum_{n_1=n_2+1}^{\infty}\left(\frac{1}{n_1-n_{k+1}} - \frac{1}{n_1}\right)\\
&= \sum_{n_2>\cdots>n_{k+1}>0} \frac{1}{n_2^{i_2}\cdots n_k^{i_k} n_{k+1}^{i_{k+1}}} \sum_{j=0}^{n_{k+1}-1} \frac{1}{n_2-j}\\
&= \sum_{n_2>\cdots>n_{k+1}>j\ge 0} \frac{1}{(n_2-j)n_2^{i_2}\cdots n_k^{i_k} n_{k+1}^{i_{k+1}}}\end{aligned}$$

or

$$S(1,i_2,\dots,i_k,i_{k+1}) = R(i_2,\dots,i_k,i_{k+1}+1). \tag{31}$$

Now we prove two results.

PROPOSITION 4.1. *For positive integers $i_1,\dots,i_k$ and a nonnegative integer i_{k+1}, the series $R(i_1,\dots,i_k)$ converges if any of $i_1,\dots,i_k$ exceeds 1, and $S(i_1,\dots,i_k,i_{k+1})$ converges if any of $i_1,\dots,i_k,i_{k+1}+1$ exceeds 1.*

PROOF. First, from (29) we have

$$S(i_1,\dots,i_k,i_{k+1}) \le S(i_1,\dots,i_k,0) \le R(i_1,\dots,i_k)$$

so that $S(i_1,\dots,i_{k+1})$ is bounded if $R(i_1,\dots,i_k)$ is. Also, if $i_1=1$ equation (31) implies $S(1,i_2,\dots,i_{k+1}) \le R(i_2,\dots,i_k,i_{k+1}+1)$, so the statement about the S's follows from the statement about the R's. To bound the R's, it suffices to treat the case where $i_1+\cdots+i_k = k+1$. Then

$$\begin{aligned}R(2,\underbrace{1,\dots,1}_{k}) &= \sum_{n_1>\cdots>n_{k+1}\ge 0} \frac{1}{n_1^2(n_1-n_{k+1})n_2\cdots n_k}\\
&\le \sum_{n_1>\cdots>n_{k+1}\ge 0,\ n_1\ge j>0} \frac{1}{n_1^2 j n_2\cdots n_k}\\
&= \zeta(3,\underbrace{1,\dots,1}_{k-1}) + k\zeta(2,\underbrace{1,\dots,1}_{k}) + \sum_{i=1}^{k-1}\zeta(2,\underbrace{1,\dots,1}_{i-1},2,\underbrace{1,\dots,1}_{k-i-1}).\end{aligned}$$

Finally, by equations (31) and (29) we have

$$R(1,2,1,\dots,1) = S(1,2,1,\dots,1,0) + \zeta(2,2,1,\dots,1) = R(2,1,\dots,1) + \zeta(2,2,1,\dots,1)$$

and similarly we can bound all the sums $R(1, \ldots, 1, 2, 1, \ldots, 1)$. $\square$

PROPOSITION 4.2. *Suppose $i_1, \ldots, i_k$ are positive integers, at least one of which exceeds 1. Then*

$$R(i_1, \ldots, i_k) - R(i_2, \ldots, i_k, i_1) = \zeta(i_1+1, i_2, \ldots, i_k) - \sum_{j=0}^{i_1-2} \zeta(i_1-j, i_2, \ldots, i_k, j+1).$$

PROOF. By the preceding result, $R(i_1, \ldots, i_k)$ converges. Now apply equation (29), then equation (30) $i_1 - 2$ times, and finally equation (31):

$$\begin{aligned} R(i_1, \ldots, i_k) &= S(i_1, \ldots, i_k, 0) + \zeta(i_1 + 1, i_2, \ldots, i_k) \\ &= S(i_1 - 1, i_2, \ldots, i_k, 1) - \zeta(i_1, \ldots, i_k, 2) + \zeta(i_1 + 1, i_2, \ldots, i_k) = \cdots = \\ & S(1, i_2, \ldots, i_k, i_1 - 1) + \zeta(i_1 + 1, i_2, \ldots, i_k) - \sum_{j=0}^{i_1-2} \zeta(i_1 - j, i_2, \ldots, i_k, j + 1) \\ &= R(i_2, \ldots, i_k, i_1) + \zeta(i_1 + 1, i_2, \ldots, i_k) - \sum_{j=0}^{i_1-2} \zeta(i_1 - j, i_2, \ldots, i_k, j + 1). \end{aligned}$$

The conclusion then follows. $\square$

To obtain Theorem 10, note that

$$\begin{aligned} 0 = (R(i_1, \ldots, i_k) - R(i_2, \ldots, i_k, i_1)) + (R(i_2, \ldots, i_k, i_1) - R(i_3, \ldots, i_k, i_1, i_2)) \\ + \cdots + (R(i_k, i_1, \ldots, i_{k-1}) - R(i_1, \ldots, i_k)) \end{aligned}$$

and apply the preceding result to each expresssion in parentheses.

3. Cyclic derivations

In the last lecture we introduced derivations of an algebra. More generally, if $\mathcal{B}$ is a 2-sided $\mathcal{A}$-algebra (that is, you can multiply an element of $\mathcal{B}$ on either side by a element of $\mathcal{A}$ to get an element of $\mathcal{B}$) and $\delta : \mathcal{A} \to \mathcal{B}$ is a linear function, then we say that δ is a derivation if

$$\delta(pq) = \delta(p)q + p\delta(q)$$

as elements of $\mathcal{B}$ for all $p, q \in \mathcal{A}$.

Now we will define cyclic derivations (introduced by Rota, Sagan and Stein [**14**], but we use the version due to Voiculescu [**16**]). Given a (noncommutative) algebra $\mathcal{A}$, we can make $\mathcal{A} \otimes \mathcal{A}$ a 2-sided $\mathcal{A}$-algebra via

$$p(t \otimes s) = pt \otimes s, \ (t \otimes s)q = t \otimes sq$$

for any $p, q, s, t \in \mathcal{A}$. Let $\mu : \mathcal{A} \otimes \mathcal{A} \to A$ be the reverse of the multiplication on $\mathcal{A}$, i.e., $\mu(s \otimes t) = ts$. A cyclic derivation from $\mathcal{A}$ to itself is a composition $\mu\delta$, where $\delta : \mathcal{A} \to \mathcal{A} \otimes \mathcal{A}$ is a derivation. Specifically, we are interested in the case where $\mathcal{A} = \mathfrak{H}$ as in the last lecture, and $\delta = \hat{C}$ is the derivation $\mathfrak{H} \to \mathfrak{H} \otimes \mathfrak{H}$ with $\hat{C}(x) = 0$ and $\hat{C}(y) = y \otimes x$. Then, for example,

$$\begin{aligned} C(x^3yxy) = \mu(x^3(y \otimes x)xy + x^3yx(y \otimes x)) = \mu(x^3y \otimes x^2y + x^3yxy \otimes x) \\ = x^2yx^3y + x^4yxy. \end{aligned}$$

THEOREM 11. *For any monomial $w \in \mathfrak{H}^1$ that is not a power of y,*

$$\zeta(C(w) - \tau C\tau(w)) = 0.$$

In the case above, we have

$$\begin{aligned}\tau C\tau(x^3yxy) = \tau C(xyxy^3) = \\ \tau\mu(x(y \otimes x)xy^3 + xyx(y \otimes x)y^2 + xyxy(y \otimes x)y + xyxy^2(y \otimes x)) \\ = \tau\mu(xy \otimes x^2y^3 + xyxy \otimes xy^2 + xyxy^2 \otimes xy + xyxy^3 \otimes x)) \\ = \tau(x^2y^3xy + xy^2xyxy + xyxyxy^2 + x^2yxy^3) \\ = xyx^3y^2 + xyxyx^2y + x^2yxyxy + x^3yxy^2\end{aligned}$$

and so the theorem says

$$\zeta(3,4) + \zeta(5,2) = \zeta(2,4,1) + \zeta(2,2,3) + \zeta(3,2,2) + \zeta(4,2,1),$$

i.e., the result of Theorem 10 applied to the sequence $(2,4)$.

Exercise 24. Show that Theorem 11 implies Theorem 10.

Exercise 25. Contrast the derivation and cyclic derivation theorems as applied to the sequence $(3,3,\ldots,3)$ (or equivalently as applied to the monomial $(x^2y)^n$).

Now we show that Theorem 11 implies the sum theorem. Let $u = x + ty$. Then the coefficient of t^k in $xu^{n-2}y$ is the sum of monomials $w \in \mathfrak{H}^0$ with $|w| = n$ and $d(w) = k$. Also, computation shows

$$C(u^{n-1}) = (n-1)txu^{n-2}y, \quad \tau C\tau(u^{n-1}) = (n-1)xu^{n-2}y.$$

Then it follows from Theorem 11 that the coefficients of t^k and t^{k-1} in $xu^{n-2}y$ are the same: i.e., this coefficient is independent of k. In particular, the coefficient equals the constant term of $xu^{n-2}y$, which is $\zeta(n)$.

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