Analogies between identities for Multiple Zeta Values and congruences for Multiple Harmonic Sums

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Introduction

For $\mathrm{Re}(s) > 1$, the Riemann zeta function is given by

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

Thanks to Euler, we know the formula

$$\zeta(s) = \frac{(2\pi)^s |B_s|}{2\, s!} \quad \text{for } s = 2, 4, 6, 8, \ldots$$

where Bernoulli numbers $B_s \in \mathbb{Q}$ are defined by generating function

$$\frac{z}{e^z - 1} = \sum_{n=0}^{\infty} \frac{B_n}{n!}\, z^n \quad \Rightarrow \quad B_n = 1, -\frac{1}{2}, \frac{1}{6}, 0, -\frac{1}{30}, 0, \frac{1}{42}, 0, -\frac{1}{30}, \ldots.$$

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- $\zeta(3)$ is irrational [Apery, 1978];
- Infinitely many $\zeta(2n+1)$ are irrational numbers;
- Conjecture. The numbers $\pi, \zeta(3), \zeta(5), \ldots, \zeta(2n+1)$ are algebraically independent over $\mathbb{Q}$: for any $n \geqslant 1$ and for any non-zero polynomial $P \in \mathbb{Z}[x_1, \ldots, x_n]$,

$$P(\pi, \zeta(3), \zeta(5), \ldots, \zeta(2n+1)) \neq 0.$$

Definitions of MHS and MZV

Let $d \geqslant 1$ and let $\mathbf{s} = (s_1, \ldots, s_d) \in (\mathbb{N}^*)^d$.
We define the *Multiple Harmonic Sum* (MHS) as

$$H_n(s_1, \ldots, s_d) := \sum_{1 \leqslant k_1 < k_2 < \cdots < k_d \leqslant n} \frac{1}{k_1^{s_1} k_2^{s_2} \cdots k_d^{s_d}}.$$

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If $s_d \geqslant 2$, the *Multiple Zeta Value* (MZV) is given by

$$\zeta(s_1, \ldots, s_d) = \lim_{n \to \infty} H_n(s_1, \ldots, s_d).$$

We call d and $w := s_1 + \cdots + s_d$ respectively the *depth* and the *weight* of $\mathbf{s}$.

Representation of MZV as iterated integral

$$\zeta(s_1,\ldots,s_d)=\int_{0<t_w<\cdots<t_2<t_1<1}\frac{dt_1\,dt_2\cdots\,dt_w}{a_1(t_1)a_2(t_2)\cdots a_w(t_w)}$$

with $a_i(t)=\begin{cases}1-t & \text{for } i\in\{s_d,s_d+s_{d-1},\ldots,w\},\\ t & \text{otherwise.}\end{cases}$

We assign to $\mathbf{s}=(s_1,\ldots,s_d)$ the word

$$\mathbf{u}=x_0^{s_d-1}x_1x_0^{s_{d-1}-1}x_1\cdots x_0^{s_1-1}x_1$$

in non-commuting letters x_0,x_1, and we write $\zeta(\mathbf{s})=\zeta(\mathbf{u})$.

For example

$$
\begin{aligned}
\zeta(x_0x_1x_1) &= \int_0^1 \frac{dt_1}{t_1} \int_0^{t_1} \frac{dt_2}{1-t_2} \int_0^{t_2} \frac{dt_3}{1-t_3} \\
&= \int_0^1 \frac{dt_1}{t_1} \int_0^{t_1} \frac{dt_2}{1-t_2} \sum_{j=1}^{\infty} \int_0^{t_2} t_3^{j-1}\, dt_3 \\
&= \int_0^1 \frac{dt_1}{t_1} \int_0^{t_1} \frac{dt_2}{1-t_2} \sum_{j=1}^{\infty} \frac{t_2^j}{j} \\
&= \int_0^1 \frac{dt_1}{t_1} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \int_0^{t_1} \frac{t_2^{j+i-1}}{j}\, dt_2 \\
&= \int_0^1 \frac{dt_1}{t_1} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{t_1^{j+i}}{j(j+i)} \\
&= \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{1}{j(j+i)^2} = \zeta(1,2).
\end{aligned}
$$

Duality relation for MZVs

The change of variable

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

in the iterated integral, yields the *duality relation* for MZVs

$$\zeta(\mathbf{u}) = \zeta(\mathbf{u}'),$$

where $\mathbf{u}'$ is defined by transposing x_0 and x_1 in $\mathbf{u}$,

$$\mathbf{u} = x_0^{s_d-1}x_1x_0^{s_{d-1}-1}x_1 \cdots x_0^{s_1-1}x_1 \to \mathbf{u}' = x_0x_1^{s_1-1} \cdots x_0x_1^{s_{d-1}-1}x_0x_1^{s_d-1}.$$

Notice that $(\mathbf{u}')' = \mathbf{u}$.

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Notice that $(\mathbf{u}')' = \mathbf{u}$. For example

$$\zeta(\{1\}^a, 2) = \zeta(x_0 x_1^{a+1}) = \zeta(x_0^{a+1} x_1) = \zeta(a+2).$$

Shuffle product $ш$

We define a product $ш$ between words on alphabet $\{x_0, x_1\}$ which is distributive over the addition and satisfies the rules

$$1)\ \forall \mathbf{u},\ 1 \mathbin{ш} \mathbf{u} = \mathbf{u} \mathbin{ш} 1 = \mathbf{u}\ ,$$

$$2)\ \forall \mathbf{u}, \mathbf{v},\ x_i\mathbf{u} \mathbin{ш} x_j\mathbf{v} = x_i(\mathbf{u} \mathbin{ш} x_j\mathbf{v}) + x_j(x_i\mathbf{u} \mathbin{ш} \mathbf{v}).$$

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$$\begin{aligned} x_0x_1 \,ш\, x_0x_1 &= 2x_0(x_1 \,ш\, x_0x_1) = 2x_0x_1(1 \,ш\, x_0x_1) + 2x_0x_0(x_1 \,ш\, x_1) \\ &= 2x_0x_1x_0x_1 + 4x_0x_0x_1x_1 \end{aligned}$$

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

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2) $\forall \mathbf{u}, \mathbf{v},\ y_i\mathbf{u} * y_j\mathbf{v} = y_i(\mathbf{u} * y_j\mathbf{v}) + y_j(y_i\mathbf{u} * \mathbf{v}) + y_{i+j}(\mathbf{u} * \mathbf{v})$.

The $*$-product is commutative and associative. Moreover

$$H_n(\mathbf{u}) \cdot H_n(\mathbf{v}) = H_n(\mathbf{u} * \mathbf{v}) \quad \text{and} \quad \zeta(\mathbf{u}) \cdot \zeta(\mathbf{v}) = \zeta(\mathbf{u} * \mathbf{v}).$$

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For example

$$y_2 * y_2 = 2y_2(1 * y_2) + y_4(1 * 1) = 2y_2^2 + y_4$$

implies that

$$H_n(2)^2 = 2H_n(2,2) + H_n(4) \quad \text{and} \quad \zeta(2)^2 = 2\zeta(2,2) + \zeta(4).$$

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Dimension Conjecture [Zagier, 1993].

Set $d_0 = 1$, $d_1 = 0$, $d_2 = 1$ and

$$d_w = d_{w-2} + d_{w-3} \qquad \forall w \geqslant 3.$$

Then $\dim(\mathfrak{Z}_w) = d_w$ for $w \geqslant 2$.

It is known that $\dim(\mathfrak{Z}_w) \leqslant d_w$, but there is not a single value of $k \geqslant 5$ for which it is known that $\dim(\mathfrak{Z}_w) > 1$.

$$\mathfrak{Z}_4 = \langle \zeta(4), \zeta(1,3), \zeta(2,2), \zeta(1,1,2) \rangle.$$

The following relations hold:

$$\begin{aligned}
\zeta(2)^2 &= \left(\frac{\pi^2}{6}\right)^2 = \frac{5}{2}\left(\frac{\pi^4}{90}\right) = \frac{5}{2}\zeta(4),\\
\zeta(1,1,2) &= \zeta(4),\\
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Therefore $\mathfrak{Z}_4 = \langle \zeta(2,2) \rangle$:

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

Basis Conjecture [Hoffman, 1997].

$\mathfrak{Z}_w$ has a basis consisting of

$$\Big\{\zeta(\mathbf{s}) : |\mathbf{s}| = w, s_i \in \{2,3\} \text{ for } i \geqslant 1\Big\}.$$

$$\begin{aligned}
d_2 &= 1, \quad \mathfrak{Z}_2 = \langle \zeta(2) \rangle, \\
d_3 &= 1, \quad \mathfrak{Z}_3 = \langle \zeta(3) \rangle, \\
d_4 &= 1, \quad \mathfrak{Z}_4 = \langle \zeta(2,2) \rangle, \\
d_5 &= 2, \quad \mathfrak{Z}_5 = \langle \zeta(2,3), \zeta(3,2) \rangle \\
d_6 &= 2, \quad \mathfrak{Z}_6 = \langle \zeta(2,2,2), \zeta(3,3) \rangle, \\
d_7 &= 3, \quad \mathfrak{Z}_7 = \langle \zeta(2,2,3), \zeta(2,3,2), \zeta(3,2,2) \rangle, \\
d_8 &= 4, \quad \mathfrak{Z}_8 = \langle \zeta(2,2,2,2), \zeta(2,3,3), \zeta(3,2,3), \zeta(3,3,2) \rangle, \\
d_9 &= 5, \quad \mathfrak{Z}_9 = \langle \zeta(2,2,2,3), \zeta(2,2,3,2), \zeta(2,3,2,2), \\
&\qquad\qquad\qquad \zeta(3,2,2,2), \zeta(3,3,3) \rangle.
\end{aligned}$$

Some of the elements of this basis can be expressed in terms of ordinary zeta values:

$$\zeta(\{2\}^a) = (-1)^a [z^{2a+1}] \left(z \prod_{k=1}^{\infty} \left(1 - \frac{z^2}{k^2}\right)\right)$$
$$= (-1)^a [z^{2a+1}] \frac{\sin(\pi z)}{\pi} = \frac{\pi^{2a}}{(2a+1)!},$$

$$\zeta(\{2\}^a, 3, \{2\}^b) = 2 \sum_{r=1}^{a+b+1} c_{r,a,b} \zeta(2r+1) \zeta(\{2\}^{a+b+1-r})$$

where $c_{r,a,b} = (-1)^r \left(\binom{2r}{2a+2} - \left(1 - \frac{1}{4^r}\right) \binom{2r}{2b+1} \right)$.

Congruences of MHSs

[Wolstenholme, 1862] For every prime $p \geqslant 5$ we have

$$H_{p-1}(1) = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{p-1} \equiv 0 \pmod{p^2}.$$

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[Zhou-Cai, 2007] Let $s, d \geqslant 1$ and $w = sd$. For every prime $p > w + 2$ we have

$$H_{p-1}(\{s\}^d) \equiv \begin{cases} (-1)^d \dfrac{s(w+1)p^2}{2(w+2)} B_{p-w-2} \pmod{p^3} & \text{if } 2 \nmid w, \\ (-1)^{d-1} \dfrac{sp}{w+1} B_{p-w-1} \pmod{p^2} & \text{if } 2 \mid w. \end{cases}$$

Remark: by Clausen-von Staudt Theorem, the denominator of B_{2n} is the product of primes p such that $p - 1 \mid 2n$.

Relations for MHSs

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Relations for MHSs can be generated by using the stuffle product and the duality relation:

$$\begin{aligned}
H_{p-1}(s_1,\dots,s_d) &= \sum_{1\leqslant k_1<\cdots<k_d\leqslant p-1} \frac{1}{k_1^{s_1}\cdots k_d^{s_d}} \\
&= \sum_{1\leqslant k_d<\cdots<k_1\leqslant p-1} \frac{1}{(p-k_1)^{s_1}\cdots(p-k_d)^{s_d}} \\
&\equiv (-1)^{|\mathbf{s}|} H_{p-1}(s_d,\dots,s_1) \pmod{p}.
\end{aligned}$$

Identities involving binomial coefficients

More relations can be obtained by using *special* binomial identities. For example, let us consider

$$\sum_{k=1}^{n} \frac{1}{k^2} = \sum_{1 \leqslant i \leqslant j \leqslant n} \frac{(-1)^{j-1}}{ij} \binom{n}{j}.$$

Since

$$(-1)^{j-1}\binom{p}{j} = (-1)^{j-1}\frac{p}{j}\cdot\frac{(p-1)\cdots(p-(j-1))}{(j-1)!} \equiv \frac{p}{j} \pmod{p^2},$$

by the above identity , it follows that

$$H_{p-1}(2) = p \sum_{1 \leqslant i \leqslant j \leqslant p-1} \frac{1}{ij^2} = pH_{p-1}(1,2) + pH_{p-1}(3) \pmod{p^2}.$$

Hence

$$H_{p-1}(1,2) \equiv \frac{H_{p-1}(2)}{p} \equiv B_{p-3} \pmod{p}.$$

More binomial identities

[Kh. & T. Hessami Pilehrood and Tauraso, 2012]
Let $a, b \geqslant 0$, $c \geqslant 2$ and $A_{n,k} = (-1)^{k-1}\binom{n}{k}/\binom{n+k}{k}$. Then

$$
\begin{aligned}
H_n^\star(\{2\}^a, c, \{2\}^b) =& 2\sum_{k=1}^{n} \frac{A_{n,k}}{k^{2a+2b+c}} \\
&+ 4 \sum_{\substack{i+j+|\mathbf{s}|=c \\ i\geqslant 1, j\geqslant 2, |\mathbf{s}|\geqslant 0}} 2^{d(\mathbf{s})} \sum_{k=1}^{n} \frac{A_{n,k} H_{k-1}(2a+i, \mathbf{s})}{k^{2b+j}},
\end{aligned}
$$

where $d(\mathbf{s})$ is the depth of $\mathbf{s}$ and

$$
H_n^\star(s_1, \ldots, s_d) := \sum_{1\leqslant k_1\leqslant k_2\leqslant\cdots\leqslant k_d\leqslant n} \frac{1}{k_1^{s_1} k_2^{s_2} \cdots k_d^{s_d}}.
$$

Let $a, b \geqslant 0$ and let p be a prime.
Then the following congruences hold modulo p.
i) For $p > w = 2a + 2b + 1$,

$$H_{p-1}(\{2\}^a, 1, \{2\}^b) \equiv \frac{4(-1)^{a+b}(a-b)(1-1/4^{a+b})}{(2a+1)(2b+1)} \binom{w-1}{2a} B_{p-w}.$$

ii) For $p > w = 2a + 2b + 3$,

$$H_{p-1}(\{2\}^a, 3, \{2\}^b) \equiv \frac{(-1)^{a+b}(a-b)}{(a+1)(b+1)} \binom{w-1}{2a+1} B_{p-w}.$$

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$$H_{p-1}(\{2\}^a, 3, \{2\}^b) \equiv \frac{(-1)^{a+b}(a-b)}{(a+1)(b+1)} \binom{w-1}{2a+1} B_{p-w}.$$

Moreover, for any prime $p > 9$,

$$H_{p-1}(1,1,1,4) \equiv \frac{27}{16} B_{p-7} \pmod{p},$$
$$H_{p-1}(1,1,1,6) \equiv \frac{1889}{648} B_{p-9} + \frac{1}{54} B_{p-3}^3 \pmod{p}.$$

For $n \geqslant 2$, define the commutative ring

$\mathbb{Q}(n) := \{a/b \in \mathbb{Q} : a/b \text{ is reduced and if a prime } p|b \text{ then } p \leqslant n\}$,

and the $\mathbb{Q}(n)$-module $\mathbb{M}(n) := \prod_{p>n} \mathbb{Z}_p$.
Let $H(\mathbf{s}) := (H_{p-1}(\mathbf{s}) \pmod{p})_{p>n} \in \mathbb{M}(n)$ for some $n \geqslant |\mathbf{s}| + 2$.
Let $\mathfrak{H}_w$ be the submodule generated by $H(\mathbf{s})$ of weight $|\mathbf{s}| = w$.
What is the rank of $\mathfrak{H}_w$?

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Dimension Conjecture [Zagier-Zhao, 2013].

Set $r_0 = 1$, $r_1 = 0$, $r_2 = 0$ and

$$r_w = r_{w-2} + r_{w-3} \qquad \forall w \geqslant 3.$$

Then $\operatorname{rank}(\mathfrak{H}_w) = r_w$ for $w \geqslant 1$.

Basis Conjecture [Zhao, 2013].

$\mathfrak{H}_w$ has a basis consisting of

$$\left\{ H(\mathbf{s}) : |\mathbf{s}| = w, s_1 = 1, s_2 = 2, s_i \in \{2,3\} \text{ for } i \geqslant 3 \right\}.$$

For example,

$$\begin{aligned}
r_1 &= 0, & \mathfrak{H}_1 &= \langle 0 \rangle,\\
r_2 &= 0, & \mathfrak{H}_2 &= \langle 0 \rangle,\\
r_3 &= 1, & \mathfrak{H}_3 &= \langle H(1,2) \rangle,\\
r_4 &= 0, & \mathfrak{H}_4 &= \langle 0 \rangle,\\
r_5 &= 1, & \mathfrak{H}_5 &= \langle H(1,2,2) \rangle,\\
r_6 &= 1, & \mathfrak{H}_6 &= \langle H(1,2,3) \rangle,\\
r_7 &= 1, & \mathfrak{H}_7 &= \langle H(1,2,2,2) \rangle,\\
r_8 &= 2, & \mathfrak{H}_8 &= \langle H(1,2,2,3), H(1,2,3,2), H(1,1,1,4) \rangle,\\
r_9 &= 2, & \mathfrak{H}_9 &= \langle H(1,2,3,3), H(1,2,2,2,2), H(1,1,1,6) \rangle,\\
r_{10} &= 3, & \mathfrak{H}_{10} &= \langle H(1,2,2,2,3), H(1,2,2,3,2), H(1,2,3,2,2),\\
& & & \quad H(1,1,1,1,6), H(2,2,1,4,1) \rangle.
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r_7 &= 1, & \mathfrak{H}_7 &= \langle H(1,2,2,2) \rangle,\\
r_8 &= 2, & \mathfrak{H}_8 &= \langle H(1,2,2,3), H(1,2,3,2) \rangle,\\
r_9 &= 2, & \mathfrak{H}_9 &= \langle H(1,2,3,3), H(1,2,2,2,2) \rangle,\\
r_{10} &= 3, & \mathfrak{H}_{10} &= \langle H(1,2,2,2,3), H(1,2,2,3,2), H(1,2,3,2,2),\\
& & & \quad H(1,1,1,1,6), H(2,2,1,4,1) \rangle.
\end{aligned}$$

More examples of series and *similar* congruences.

The following congruences hold modulo p^3, for any prime $p > 5$,

- [Tauraso, 2010]

$$\sum_{k=1}^{\infty} \frac{1}{k^2}\binom{2k}{k}^{-1} = \frac{1}{3}\,\zeta(2), \qquad \sum_{k=1}^{p-1} \frac{1}{k^2}\binom{2k}{k}^{-1} \equiv \frac{1}{3}\,\frac{H_{p-1}(1)}{p},$$

$$\sum_{k=1}^{\infty} \frac{(-1)^k}{k^3}\binom{2k}{k}^{-1} = -\frac{2}{5}\,\zeta(3), \quad \sum_{k=1}^{p-1} \frac{(-1)^k}{k^3}\binom{2k}{k}^{-1} \equiv \frac{2}{5}\,\frac{H_{p-1}(1)}{p^2}.$$

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- [Mattarei-Tauraso, 2012]

$$\sum_{k=1}^{\infty} \frac{(-1)^k}{k}\binom{2k}{k}^{-1} = -\frac{2\sqrt{5}\ln(\phi)}{5},$$

$$p\sum_{k=1}^{p-1} \frac{(-1)^k}{k}\binom{2k}{k}^{-1} \equiv \frac{1-L_pF_p}{2} - \frac{2\sqrt{5}\pounds_2(\phi)}{5}\,p^2,$$

where $\phi = \frac{1+\sqrt{5}}{2}$ and $\pounds_2(x) = \sum_{k=1}^{p-1} \frac{x^k}{k^2}$.


That's all Folks!