

# Multiple zeta values and modular forms

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# Outline

1 Introduction, definitions and motivation

2 Algebraic properties

3 Modular forms relations

( +  $\varepsilon$  of new work with Adam Keilthy?)

## Introduction, definitions and motivation

# Riemann zeta values

## Definition (Riemann zeta function)

The **Riemann zeta function** is

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}, \quad \operatorname{Re}(s) > 1$$

Special values?

$$\zeta(2) = \frac{\pi^2}{6}, \quad \zeta(4) = \frac{\pi^4}{90}, \quad \zeta(6) = \frac{\pi^6}{945}, \quad \dots$$

## Euler (1730's)

The following holds:

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

where  $\sum_{k=0}^{\infty} B_k \frac{x^k}{k!} := \frac{x}{e^x - 1}$  defines the **Bernoulli number**  $B_k$ .

# Questions about $\zeta(n)$

- What is known about  $\zeta(3)$ ?
  - No evaluation known, numerically it seems  $\zeta(3)\pi^{-3} \notin \mathbb{Q}$
  - Know that  $\zeta(3) \notin \mathbb{Q}$  (Apéry, 1978)
- What is known about  $\zeta(5)$ ?
  - At least one of  $\zeta(5), \zeta(7), \zeta(9), \zeta(11)$  irrational. (Zudilin, further work by Ball, Rivoal)  
(But which ones?)

## Idea

To try to understand  $\zeta(n)$ , fit it into a (bigger) algebraic structure

# Multiple zeta values (MZV's)

## Definition

The **multiple zeta value**  $\zeta(k_1, k_2, \dots, k_d)$  is defined by

$$\zeta(k_1, k_2, \dots, k_d) = \sum_{1 \leq n_1 < n_2 < \dots < n_d} \frac{1}{n_1^{k_1} n_2^{k_2} \dots n_d^{k_d}}$$

- Convergence:  $k_d > 1$
- The **weight** is  $k_1 + \dots + k_d$ , the **depth** is  $d$

## Motivation

Product

$$\zeta(a)\zeta(b) = \zeta(a, b) + \zeta(b, a) + \zeta(a + b)$$

# Appearances

Appears in many areas

- Vassiliev knot invariants
- Dirichlet eigenvalues of regular polygons
- Scattering amplitudes in high-energy physics
- Number theory
- ...

## Algebraic properties



# Relations

MZV's satisfy many relations

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

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

$$\sum_{\substack{i+j+k=n \\ k>1}} \zeta(i, j, k) = \zeta(n)$$

$$28\zeta(3, 9) + 150\zeta(5, 7) + 168\zeta(7, 5) = \frac{5197}{691}\zeta(12)$$

## Dimensions

By eliminating linearly dependent elements (numerically, via LLL), we find candidate dimensions

weight $w$	1	2	3	4	5	6	7	8	9	10	11	12
$d_k = \dim_{\mathbb{Q}}$	0	1	1	1	2	2	3	4	5	7	9	12

Conjecture:  $d_k = d_{k-2} + d_{k-3}$ .

# Stuffle product

Multiply series

$$\begin{aligned} \zeta(a, b)\zeta(c) &= \sum_{0 < i < j} \frac{1}{i^a j^b} \sum_{0 < k} \frac{1}{k^c} \\ &= \left( \sum_{0 < i < j < k} + \sum_{0 < i < k < j} + \sum_{0 < k < i < j} + \sum_{0 < i < j = k} + \sum_{0 < i = k < j} \right) \frac{1}{i^a j^b k^c} \\ &= \zeta(a, b, c) + \zeta(a, c, b) + \zeta(c, a, b) + \zeta(a, b + c) + \zeta(a + c, b) \end{aligned}$$

More formally

## Definition (Stuffle product)

For words  $w, v$  in letters  $z_i$ , recursively define

$$z_a w * z_b v = z_a (w * z_b v) + z_b (z_a w * v) + z_{a+b} (w * v)$$

This encodes  $\zeta(n_1, \dots, n_d)\zeta(m_1, \dots, m_e)$  via  $\zeta(z_{n_1} \cdots z_{n_d}) = \zeta(n_1, \dots, n_d)$ .

# Integral representation

## Proposition

$$\zeta(n_1, \dots, n_d) = (-1)^d I(0; 1, \{0\}^{n_1-1}, 1, \{0\}^{n_2-1}, \dots, 1, \{0\}^{n_d-1}; 1)$$

where

$$I(x_0; x_1, \dots, x_N; x_{N+1}) = \int_{0 < t_1 < \dots < t_N < 1} \frac{dt}{t_1 - x_1} \dots \frac{dt}{t_n - x_n}$$

Proof idea: expand geometric series

$$\begin{aligned} \int_{0 < t_1 < t_2 < 1} \frac{dt_1}{1 - t_1} \frac{dt_2}{t_2} &= \sum_{n_1=1}^{\infty} \int_{0 < t_1 < t_2 < 1} t_1^{n_1} dt_1 \frac{dt_2}{t_2} \\ &= \sum_{n_1=1}^{\infty} \int_{0 < t_2 < 1} \frac{t_2^{n_1-1}}{n_1} dt_2 = \sum_{n_1=1}^{\infty} \frac{1}{n_1^2} = \zeta(2) \end{aligned}$$

## Corollary (Duality)

$$\zeta(n_1, \dots, n_d) \approx 10^{n_1-1} \dots 10^{n_d-1} \xleftrightarrow[\text{reverse}]{0 \leftrightarrow 1} 10^{m_1-1} \dots 10^{m_e-1} \approx \zeta(m_1, \dots, m_e)$$

# Shuffle product

Multiply integrals for  $\zeta(2)\zeta(2)$

$$\begin{aligned} & \int_{0 < t_1 < t_2 < 1} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \cdot \int_{0 < s_1 < s_2 < 1} \frac{ds_1}{1-s_1} \frac{ds_2}{s_2} = \int_{\text{shuffles}} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \frac{ds_1}{1-s_1} \frac{ds_2}{s_2} \\ & = 4 \int_{0 < t_1 < t_2 < t_3 < t_4} \frac{dt_1}{1-t_1} \frac{dt_2}{1-t_2} \frac{dt_3}{t_3} \frac{dt_4}{t_4} + 2 \int_{0 < t_1 < t_2 < t_3 < t_4} \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \frac{dt_3}{1-t_3} \frac{dt_4}{t_4} \\ & = 4\zeta(1, 3) + 2\zeta(2, 2) \end{aligned}$$

More formally

## Definition (Shuffle product)

For words  $w, v$  in letters  $e_0, e_1$ , recursively define

$$e_i w \sqcup e_j v = e_j (w \sqcup e_i v) + e_i (e_j w \sqcup v)$$

This encodes  $\zeta(n_1, \dots, n_d)\zeta(m_1, \dots, m_e)$  via  $\zeta(e_{i_1} \cdots e_{i_n}) = \pm I(0; e_{i_1}, \dots, e_{i_n}; 1)$ .

# Double shuffle relations

## Compare product structures

The shuffle- and stuffle-product give two *different* algebra structures on MZV's!

## Example

$$2\zeta(2, 2) + \zeta(4) \stackrel{*}{=} \zeta(2)\zeta(2) \stackrel{\sqcup}{=} 4\zeta(1, 3) + 2\zeta(2, 2) \quad \Longrightarrow \quad \zeta(1, 3) = \frac{1}{4}\zeta(4)$$

Allow regularisation  $\zeta(1) =: T$  (a formal object); can extend  $*, \sqcup$

## Conjecture

*Comparing  $\zeta(\underline{\mathbf{k}})\zeta(\underline{\mathbf{l}})$  via shuffle product and stuffle gives all MZV relations.*

## Warning

- Need regularisation to get  $\zeta(1, 2) = \zeta(3)$
- Difficult to deduce given relations (need nice structure, or big linear algebra)

# Double shuffle relations for double zetas

In weight  $k$ , the shuffle and stuffle product give double zeta relations

$$\zeta(a)\zeta(b) = \zeta(a, b) + \zeta(b, a) - \zeta(k)$$

$$\zeta(a)\zeta(b) = \sum_{r+s=k} \left[ \binom{r-1}{a-1} + \binom{r-1}{b-1} \right] \zeta(r, s)$$

Introduce generating series

$$P(X, Y) = \sum_{r+s=k} \zeta(r)\zeta(s)X^{r-1}Y^{s-1}$$

$$Z(X, Y) = \sum_{r+s=k} \zeta(r, s)X^{r-1}Y^{s-1}$$

Then we get

$$Z(X, Y) + Z(Y, X) = P(X, Y) - \zeta(k) \frac{X^{k-1} - Y^{k-1}}{X - Y}$$

$$Z(X + Y, Y) + Z(X + Y, X) = P(X, Y)$$

## Modular forms relations

# Modular forms connections

Recall Eisenstein series (in some normalisation):

$$G_k(z) = \frac{1}{2} \sum'_{p,q \in \mathbb{Z}} \frac{1}{(p\tau + q)^k} = \zeta(k) + \sum_{n=1}^{\infty} \sigma_k(n) q^n$$

## Constant term relations

Relations

$$\sum c_a G_a(z) G_{k-a}(z) = c_0 G_k(z)$$

give relations for zetas

$$\sum c_a \zeta(a) \zeta(k-a) = c_0 \zeta(k)$$

by taking constant term.

(More interesting relations from cusp forms!)



# Period polynomials

Given a cusp form  $f \in S_{2k}(\mathrm{SL}_2(\mathbb{Z}))$ , consider the *period* polynomial

$$\begin{aligned} r(f)(X, Y) &= \int_0^{i\infty} f(t) Y^{2k-2} (X/Y - t)^{2k-2} dt \\ &= \sum_{n=0}^w i^{1-n} \binom{w}{n} X^{2k-2-n} Y^n r_n(f) \end{aligned}$$

where the  $r$ -th period is

$$r_n(f) = \int_0^\infty f(it) t^n dt, \quad 0 \leq n \leq 2k - 2$$

## Fact

Up to multiplying by a single (transcendental) number, the  $X^{\text{even}}Y^{\text{even}}$  part is in  $\mathbb{Q}[X, Y]$ . Similarly the  $X^{\text{odd}}Y^{\text{odd}}$  part.

# Eichler-Shimura

Matrix  $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in (\mathbb{P})\mathrm{SL}_2(\mathbb{Z})$  acts on homogeneous polynomials  $f(X, Y)$  of degree  $k$  via

$$(P|_{\gamma})(X, Y) = (cX + dY)^k P(aX + bY, cX + dY)$$

## Period polynomial subspace

Since  $\int_0^{i\infty} + \int_{i\infty}^0 = 0$  and  $\int_0^{i\infty} + \int_{i\infty}^1 + \int_1^0 = 0$ , period polynomials  $P = r(f)(X, Y)$  have special properties

$$\begin{aligned} P + P|_S &= 0 & S &= \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \\ P + P|_U + P|_{U^2} &= 0 & U &= \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

## Theorem (Eichler-Shimura, very rough)

*Period polynomials of degree  $k$  are isomorphic to cusp forms of weight  $k$*

# Double shuffle, revisited

Double-zeta double shuffle relations are

$$Z(X+Y, Y) + Z(X+Y, X) - Z(X, Y) - Z(Y, X) - \zeta(k) \frac{X^{k-1} - Y^{k-1}}{X - Y} = 0$$

Can construct general solutions (realisations, with  $\zeta(k) \rightarrow 0$ ) to these relations via

$$Z(X, Y) = A(X, Y) - A(X, X - Y) + A(Y, Y - X)$$

for  $A(X, Y)$  any polynomial even with respect to  $Y$ . Can use ideas like this to connect to period polynomials.

## Theorem (Gangl-Kaneko-Zagier, 2006)

Let  $f \in S_{w+2}(\mathrm{SL}_2(\mathbb{Z}))$ , with (even part) of period polynomial  $P_f(X, Y)$ , and define  $a_r$  by

$$\sum_{r=0}^w a_r X^r Y^{w-r} = P_f(X + Y, X).$$

Then

$$\sum_{\substack{r=0 \\ \text{even}}}^{w-2} a_r r! (w-r)! \zeta(r+1, w+1-r) \in \mathbb{Q} \zeta(w+2)$$

# Examples

Weight 12, have one degree 10 period polynomial

$$P_f(X, Y) = -X^8Y^2 + 3X^6Y^4 - 3X^4Y^6 + X^2Y^8$$

$$P_f(X + Y, X) = \cancel{-8X^7Y^3} - 28X^6Y^4 - \cancel{38X^5Y^5} - 25X^4Y^6 - \cancel{8X^3Y^7} - X^2Y^8$$

$$\text{Relation: } -28 \cdot 4!6!\zeta(7, 5) - 25 \cdot 4!6!\zeta(5, 7) - 2!8!\zeta(3, 9) = -4!5! \cdot \frac{5197}{691}\zeta(12)$$

Weight 16, only one degree 14 period polynomial

$$P_f(X, Y) = -2X^{12}Y^2 + 7X^{10}Y^4 - 11X^8Y^6 + 11X^6Y^8 - 7X^4Y^{10} + 2X^2Y^{12}$$

$$P_f(X + Y, X) \rightsquigarrow -132X^{10}Y^4 - 675X^8Y^6 - 686X^6Y^8 - 125X^4Y^{10} - 2X^2Y^{12} + \cancel{X^{\text{odd}}Y^{\text{odd}}}, s$$

$$\begin{aligned} \text{Relation: } & -2 \cdot 2!12!\zeta(3, 13) - 125 \cdot 4!10!\zeta(5, 11) - 686 \cdot 6!8!\zeta(7, 9) \\ & - 675 \cdot 6!8!\zeta(9, 7) - 132 \cdot 4!10!\zeta(11, 5) = -6!8! \cdot \frac{78967}{3617}\zeta(12) \end{aligned}$$

# Propagation of modular relations

## Theorem (C-Keilthy, 2022?, Schematic)

*Following evaluation holds modulo products*

$$\zeta(\overbrace{\{2\}^a},^{2, \dots, 2 \text{ repeated } a \text{ times}}, 4, \{2\}^b) = 4(-1)^n \left[ -\zeta(2a+2, 2b+2) - \zeta(2a+3, 2b+1) \right. \\ \left. + \sum_{j=1}^{2n+3} 2^{j-4-2n} \left( \binom{2n+3-j}{2b+1} - \binom{2n+3-j}{2a+1} \right) \zeta(j, 2n+4-j) \right]$$

## Corollary

*Modulo products,*

$$\sum_{i=a}^{n-a} \zeta(\{2\}^i, 4, \{2\}^{n-i}) = 4(-1)^n \zeta(2a+1, 2n-2a+3).$$

So the modular relations propagate to  $\zeta(2, \dots, 2, 4, 2, \dots, 2)$ .

# Summary

- Definition of multiple zeta values
- Appears throughout physics/math
- Integral representation and duality
- Shuffle and stuffle product
  - double shuffle relations
  - (need for) regularisation
- Period polynomials
- Double zeta relations from cusp forms
  - Explicit recipe from period polynomials
- Modular relations for  $\zeta(2, \dots, 2, 4, 2, \dots, 2)$