Multiple Zeta Values and Multiple Apéry-Like Sums

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Multiple zeta values

Riemann zeta function

The Riemann zeta function $\zeta(s)$, is a function of a complex variable s that analytically continues the sum of the Dirichlet series

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

When $Re(s) > 1$.

Riemann zeta function at even positive integers

We know that

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

For odd positive integers, no such simple expression is known

Euler's classical formula

Euler's classical formula

$$\zeta(2) = 3 \sum_{m=1}^{\infty} m^{-2} \binom{2m}{m}^{-1}$$

Apéry like function

$$\sigma(s) = \sum_{n=1}^{\infty} \binom{2n_1}{n_1}^{-1} \frac{1}{n^s}$$

We have the classical results

$$\zeta(2) = 3\sigma(2), \quad \zeta(4) = \frac{36}{17}\sigma(4)$$

Question?

Weather we can generalization of Euler's classical formula for positive integers $\geqslant 2$

Answer: yes we can

In My papper

Double tails of multiple zeta values, Journal of Number Theory 170 (2017) 228-249

I have a generalization of Euler's classical formula $\zeta(2) = 3\sum_{m=1}^{\infty} m^{-2} \binom{2m}{m}^{-1}$ to all multiple zeta values

This work I have done under the guidence of Professor J. Oesterlé

Notations

$\mathbf{N}$ denotes the set of non-negative integers

A finite sequence $\mathbf{a} = (a_1, \ldots, a_r)$ of positive integers is called *a composition*

The integer r is called *the depth* of $\mathbf{a}$ and the integer $k = a_1 + \ldots + a_r$ *the weight* of $\mathbf{a}$

Admissible Composition

Composition **a** is said to be *admissible* if either $r \geqslant 1$ and $a_1 \geqslant 2$, or **a** is the empty composition denoted $\varnothing$

Multiple zeta values

To each admissible composition $\mathbf{a} = (a_1, \ldots, a_r)$, one associates a real number $\zeta(\mathbf{a})$. It is defined by the convergent series

$$\zeta(\mathbf{a}) = \sum_{n_1 > \ldots > n_r > 0} n_1^{-a_1} \ldots n_r^{-a_r}. \tag{1}$$

when $r \geqslant 1$, and by $\zeta(\varnothing) = 1$ when $r = 0$. These numbers are called *multiple zeta values* or *Euler-Zagier numbers*.

Binary word

A *binary word* is by definition a word w constructed on the alphabet $\{0, 1\}$. Its letters are called *bits*

The number of bits of w is called *the weight* of w and denoted by $|w|$

The number of bits of w equal to 1 is called *the depth* of w

Composition to Binary word

To any composition $\mathbf{a} = (a_1, \ldots, a_r)$, one associates the binary word

$$\mathbf{w}(\mathbf{a}) = \{0\}_{a_1-1}1 \ldots \{0\}_{a_r-1}1 \tag{2}$$

where for each integer $u \geqslant 0$, $\{0\}_u$ denotes the binary word consisting of u bits equal to 0, and where $\mathbf{w}(\mathbf{a})$ is the empty word if $\mathbf{a}$ is the empty composition

Binary word

We shall denote by W the set of binary words. When $\varepsilon, \varepsilon' \in \{0, 1\}$, ${}_{\varepsilon}\mathrm{W}$ and $\mathrm{W}_{\varepsilon'}$ denote the sets of binary words starting by ε and ending by ε' respectively, and ${}_{\varepsilon}\mathrm{W}_{\varepsilon'}$ their intersection.

Admissible word

The map **w** is a bijection from the set of compositions onto the set of binary words not ending by 0. Non empty compositions correspond to words in W_1, and non empty admissible compositions to words in ${}_0\mathrm{W}_1$. Therefore a binary word will be called *admissible* if either it belongs to ${}_0\mathrm{W}_1$, or it is empty.

Maxim Kontsevich's iterated integral expression for MZV

Maxim Kontsevich has discovered that for each admissible composition $\mathbf{a}$, the multiple zeta value $\zeta(\mathbf{a})$ can be written as an iterated integral.
More precisely, if $w = \varepsilon_1 \dots \varepsilon_k$ denotes the associated binary word $\mathbf{w}(\mathbf{a})$, we have

$$\begin{aligned} \zeta(\mathbf{a}) &= \mathrm{It}\int_0^1 (\omega_{\varepsilon_1}, \dots, \omega_{\varepsilon_k}) \qquad (3) \\ &= \int_{1>t_1>\dots>t_k>0} f_{\varepsilon_1}(t_1)\dots f_{\varepsilon_k}(t_k) dt_1 \dots dt_k \end{aligned}$$

where $\omega_i = f_i(t)dt$, with $f_0(t) = \frac{1}{t}$ and $f_1(t) = \frac{1}{1-t}$.

Duality relations

Dual word and dual composition

Let $w = \varepsilon_1 \ldots \varepsilon_k$ be a binary word. Its *dual word* is defined to be $\overline{w} = \bar{\varepsilon}_k \ldots \bar{\varepsilon}_1$, where $\overline{0} = 1$ and $\overline{1} = 0$.

When w is admissible, so is $\overline{w}$. We can therefore define the *dual composition* of an admissible composition $\mathbf{a}$ to be the admissible composition $\overline{\mathbf{a}}$ such that $\mathbf{w}(\overline{\mathbf{a}})$ is dual to $\mathbf{w}(\mathbf{a})$. When $\mathbf{a}$ has weight k and depth r, $\overline{\mathbf{a}}$ has weight k and depth $k - r$.

duality relation

For any admissible composition $\mathbf{a}$, we have

$$\zeta(\mathbf{a}) = \zeta(\overline{\mathbf{a}}) \tag{4}$$

This we can prove by By the change of variables $t_i \mapsto 1 - t_{k+1-i}$ in the integral (3),

Tail and double tail of multiple zeta values

Tail of multiple zeta values

When **a** is a non empty admissible composition, we can define for each integer $n \geqslant 0$ *the n-tail* of the series (1) to be the sum of the series

$$\sum_{n_1 > \ldots > n_r > n} n_1^{-a_1} \ldots n_r^{-a_r}. \tag{5}$$

Integral formula for tail of multiple zeta values

This n-tail can be written as the iterated integral

$$\mathrm{It}\int_0^1 (\omega_{\varepsilon_1}, \ldots, t^n \omega_{\varepsilon_k}) = \int_{1>t_1>\ldots>t_k>0} f_{\varepsilon_1}(t_1)\ldots f_{\varepsilon_k}(t_k) t_k^n dt_1 \ldots dt_k \tag{6}$$

where $\varepsilon_1 \ldots \varepsilon_k$ is the binary word $\mathbf{w}(\mathbf{a})$

Double tail of multiple zeta values

Definition

— *When* **a** *is a non empty admissible composition, we define for* m *and* n *in* $\mathbf{N}$ *the* (m,n)*-double tail* $\zeta(\mathbf{a})_{m,n}$ *of* $\zeta(\mathbf{a})$ *as the iterated integral*

$$\begin{aligned} \zeta(\mathbf{a})_{m,n} &= \mathrm{It}\int_0^1 ((1-t)^m \omega_{\varepsilon_1}, \ldots, t^n \omega_{\varepsilon_k}) \qquad (7) \\ &= \int_{1>t_1>\ldots>t_k>0} (1-t_1)^m f_{\varepsilon_1}(t_1) \ldots f_{\varepsilon_k}(t_k) t_k^n dt_1 \ldots dt_k \,, \end{aligned}$$

where $\varepsilon_1 \ldots \varepsilon_k$ *is the binary word* $\mathbf{w}(\mathbf{a})$.

Series expression for Double tail of MZV

Theorem

— *Let* $\mathbf{a} = (a_1, \ldots, a_r)$ *be a non empty admissible composition. For all* m *and* n *in* $\mathbf{N}$*, the* (m, n)*-double tail of* $\zeta(\mathbf{a})$ *is given by the convergent series*

$$\zeta(\mathbf{a})_{m,n} = \sum_{n_1 > \ldots > n_r > n} \binom{n_1 + m}{m}^{-1} n_1^{-a_1} \ldots n_r^{-a_r}. \tag{8}$$

Duality relation for double tails

THEOREM

— *Let* $\mathbf{a}$ *be a non empty admissible composition and* $\overline{\mathbf{a}}$ *denote its dual composition. For any* m *and* n *in* $\mathbf{N}$*, we have*

$$\zeta(\mathbf{a})_{m,n} = \zeta(\overline{\mathbf{a}})_{n,m} \tag{9}$$

Conceptually very simple, Example

Note that $\zeta(\mathbf{a})_{0,n}$ is nothing but the usual n-tail of $\zeta(\mathbf{a})$. Formula (9) tells us that it is equal $\zeta(\overline{\mathbf{a}})_{n,0}$.

This equality is in fact the main theorem of a recent paper by J. M. Borwein and O-Yeat Chan (*Duality in tails of multiple zeta values*, th. 14,Int. J. Number Theory **6** (2010), 501-514), for which Theorem 2 therefore provides a conceptually very simple proof.

Upper bounds of double tails of multiple zeta values

Upper bounds double tails

Theorem

— *Let* $\mathbf{a}$ *be a non empty admissible composition. For all* m *and* n *in* $\mathbf{N}$*, we have*

$$\zeta(\mathbf{a})_{m,n} \leqslant \frac{m^m n^n}{(m+n)^{m+n}} \zeta(\mathbf{a}), \tag{10}$$

and $\zeta(\mathbf{a}) \leqslant \frac{\pi^2}{6}$*. We have in particular*

$$\zeta(\mathbf{a})_{n,n} \leqslant 2^{-2n} \zeta(\mathbf{a}) \leqslant 2^{-2n} \frac{\pi^2}{6}. \tag{11}$$

Upper bound comparison - Tail and double tail

$\zeta(\mathbf{a})_n$ is equivalent to

$$\frac{n^{r-(a_1+\ldots+a_r)}}{(a_1-1)(a_1+a_2-2)\ldots(a_1+\ldots+a_r-r)} \tag{12}$$

when n tends to $+\infty$.

Now we can understand symmetric double tail is much smaller than tail

Double tail Definition

DEFINITION

— *Let* $w = \varepsilon_1 \dots \varepsilon_k$ *be a binary word and let* $m, n \in \mathbf{N}$*. Assume* $m \geqslant 1$ *when* $w \in {}_1\mathrm{W}$*, and* $n \geqslant 1$ *when* $w \in \mathrm{W}_0$*. We define a real number* $\zeta(w)_{m,n}$ *by the convergent iterated integral*

$$\zeta(w)_{m,n} = \mathrm{It}\int_0^1 ((1-t)^m \omega_{\varepsilon_1}, \dots, t^n \omega_{\varepsilon_k}), \tag{13}$$

when $k \geqslant 2$*,*

Double tail Definition

and in the remaining cases by

$$\zeta(0)_{m,n} = \int_0^1 (1-t)^m t^n \frac{dt}{t} = \frac{m!(n-1)!}{(m+n)!}\,, \tag{14}$$

$$\zeta(1)_{m,n} = \int_0^1 (1-t)^m t^n \frac{dt}{1-t} = \frac{(m-1)!n!}{(m+n)!}\,, \tag{15}$$

$$\zeta(\varnothing)_{m,n} = \frac{m!\,n!}{(m+n)!}. \tag{16}$$

Recurrence formula

Recurrence formula

THEOREM

— *Let w be a binary word and and let $m, n \in \mathbf{N}$.*
a) Assume $n \geqslant 1$. Then we have

$$\begin{cases} \zeta(w0)_{m,n} = n^{-1}\zeta(w)_{m,n} & \text{if} m \geqslant 1 \text{ or } w \notin {}_1\mathrm{W}, \\ \zeta(w1)_{m,n-1} = \zeta(w1)_{m,n} + n^{-1}\zeta(w)_{m,n} & \text{if } m \geqslant 1 \text{ or } w \in {}_0\mathrm{W} \end{cases} \tag{17}$$

Recurrence formula

THEOREM

b) Assume $m \geqslant 1$. Then we have

$$\begin{cases} \zeta(1w)_{m,n} = m^{-1}\zeta(w)_{m,n} & \text{if } n \geqslant 1 \text{ or } w \notin \mathrm{W}_0 \\ \zeta(0w)_{m-1,n} = \zeta(0w)_{m,n} + n^{-1}\zeta(w)_{m,n} & \text{if } n \geqslant 1 \text{ or } w \in \mathrm{W}_1 \end{cases} \tag{18}$$

Recurrence relations

Initial, Middle, Final words

Let w be an non empty admissible binary word. There exists a unique triple (v, a, b), where v is an admissible binary word, empty or not, and a, b are positive integers, such that $w = 0\{1\}_{b-1}v\{0\}_{a-1}1$.

$w^{\mathrm{init}} = 0\{1\}_{b-1}v$, $w^{\mathrm{fin}} = v\{0\}_{a-1}1$ and $w^{\mathrm{mid}} = v$.

Recurrence relations

Theorem

— *Let w be an non empty admissible binary word. Then we have*

$$\begin{aligned} \zeta(w)_{n-1,n-1} &= \zeta(w)_{n,n} + n^{-a}\zeta(w^{\mathrm{init}})_{n,n} + n^{-b}\zeta(w^{\mathrm{fin}})_{n,n} \\ &+ n^{-a-b}\zeta(w^{\mathrm{mid}})_{n,n} \end{aligned} \tag{19}$$

An algorithm to compute multiple zeta values

An algorithm to compute multiple zeta values

- Let $w = \varepsilon_1 \dots \varepsilon_k$ be a non empty admissible binary word.
- Let V denote the set of non empty admissible subwords of w.
- We set $u_{\mathrm{N}}(v) = 0$ for all $v \in \mathrm{V}$.

An algorithm to compute multiple zeta values

- Compute inductively $u_n(v)$ for $v \in \mathrm{V}$, when n is decreasing from N to 0, by using the recurrence relation

$$\begin{aligned} u_{n-1}(v) &= u_n(v) + n^{-a(v)} u_n(v^{\mathrm{init}}) + n^{-b(v)} u_n(v^{\mathrm{fin}}) \\ &+ n^{-a(v)-b(v)} u_n(v^{\mathrm{mid}}) \end{aligned} \tag{20}$$

- $a(v) = |v| - |v^{\mathrm{init}}|$, $b(v) = |v| - |v^{\mathrm{fin}}|$,
- in case $v^{\mathrm{init}} = 0$, $v^{\mathrm{fin}} = 1$ or $v^{\mathrm{mid}} = \varnothing$, the corresponding value $u_n(0)$, $u_n(1)$ or $u_n(\varnothing)$ is taken to be $\zeta(0)_{n,n}$, $\zeta(1)_{n,n}$ or$\zeta(\varnothing)_{n,n}$, as defined by formula (14), (15) or (16) respectively

implementation details

I first implemented this algorithm in the language Python 2.7.5 on my personal computer. As an example, computing the 127 multiple zeta values corresponding to admissible compositions of weight $\leqslant 8$ with 1000 exact decimal digits took 5 minutes and 9 seconds. With only 100 exact decimal digits, it took 5.8 seconds. The same computations have been implemented by Henri Cohen in Pari/GP and in C , which have the advantage of being interpreted languages. They then take 0.9 seconds and 0.006 seconds respectively.

Error Estimates

PROPOSITION

The theoretical error $|\zeta(v) - u_0(v)|$ *in the previous algorithm is bounded above by* $2^{-2\mathrm{N}}(\mathrm{N}+1)^2\frac{\pi^2}{6}$ *for each* $v \in \mathrm{V}$. *If at each step of the algorithm the right hand side of* (35) *is computed to an accuracy at most* α, *the total error (theoretical error plus rounding errors) is bounded above by* $2^{-2\mathrm{N}}(\mathrm{N}+1)^2\frac{\pi^2}{6} + \frac{\mathrm{N}(\mathrm{N}+1)(2\mathrm{N}+1)}{6}\alpha$.

Some examples

In weight 2

$w = 01$, corresponding to the composition (2).

$w^{\mathrm{init}} = 0$, $w^{\mathrm{fin}} = 1$ and $w^{\mathrm{mid}} = \varnothing$, and for each integer $n \geqslant 1$, the recurrence relation expressed in terms of words

$$\begin{aligned} \zeta(01)_{n-1,n-1} &= \zeta(01)_{n,n} + n^{-1}\zeta(0)_{n,n} + n^{-1}\zeta(1)_{n,n} + n^{-2}\zeta(\varnothing)_{n,n} \\ &= \zeta(01)_{n,n} + 3n^{-2}\zeta(\varnothing)_{n,n}\,, \end{aligned} \tag{21}$$

Some examples

or equivalently, in term of compositions,

$$\zeta(2)_{n-1,n-1} = \zeta(2)_{n,n} + 3n^{-2}\zeta(\varnothing)_{n,n}\,, \tag{22}$$

where $\zeta(\varnothing)_{n,n} = \binom{2n}{n}^{-1}$. We therefore have, for all integers $n \geqslant 0$,

$$\zeta(2)_{n,n} = 3\sum_{m=n+1}^{\infty} m^{-2}\binom{2m}{m}^{-1}. \tag{23}$$

This yields in particular for $n = 0$ the following formula, due to Euler :

$$\zeta(2) = 3\sum_{m=1}^{\infty} m^{-2}\binom{2m}{m}^{-1}. \tag{24}$$

Some examples

In weight 4

$$\mathrm{X}_{n-1} = \mathrm{X}_n + \mathrm{A}\mathrm{Y}_n, \tag{25}$$

where

$$\mathrm{X}_n = \begin{pmatrix} \zeta(4)_{n,n} \\ \zeta(3,1)_{n,n} \\ \zeta(2,2)_{n,n} \end{pmatrix}, \quad \mathrm{A} = \begin{pmatrix} 1 & 0 & 2 \\ 2 & 1 & 0 \\ 0 & 2 & 1 \end{pmatrix}, \quad \mathrm{Y}_n = \begin{pmatrix} n^{-1}\zeta(3)_{n,n} \\ n^{-2}\zeta(2)_{n,n} \\ n^{-4}\zeta(\varnothing)_{n,n} \end{pmatrix}.$$

Some examples

In weight 6

$$\mathrm{X}_n = \begin{pmatrix} \zeta(6)_{n,n} \\ \zeta(5,1)_{n,n} \\ \zeta(4,2)_{n,n} \\ \zeta(4,1,1)_{n,n} \\ \zeta(3,3)_{n,n} \\ \zeta(3,2,1)_{n,n} \\ \zeta(3,1,2)_{n,n} \\ \zeta(2,4)_{n,n} \\ \zeta(2,2,2)_{n,n} \\ \zeta(2,1,3)_{n,n} \end{pmatrix}, \quad \mathrm{A} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 1 \end{pmatrix}, \quad \mathrm{Y}_n = \begin{pmatrix} n^{-1}\zeta(5)_{n,n} \\ n^{-1}\zeta(4,1)_{n,n} \\ n^{-1}\zeta(3,2)_{n,n} \\ n^{-1}\zeta(2,3)_{n,n} \\ n^{-2}\zeta(4)_{n,n} \\ n^{-2}\zeta(3,1)_{n,n} \\ n^{-2}\zeta(2,2)_{n,n} \\ n^{-3}\zeta(3)_{n,n} \\ n^{-4}\zeta(2)_{n,n} \\ n^{-6}\zeta(\varnothing)_{n,n} \end{pmatrix}.$$

Further notations

we extend these types of formulas to all multiple zeta values. To state our result, we shall need some further notations. For any non empty composition $\mathbf{a} = (a_1, \ldots, a_r)$ (admissible or not) and any integer $m \geqslant 1$, we define a real number $\varphi_m(\mathbf{a})$ by the finite sum

$$\varphi_m(\mathbf{a}) = m^{-a_1} \sum_{m > n_2 > \ldots > n_r > 0} n_2^{-a_2} \ldots n_r^{-a_r}, \qquad (26)$$

Further notations

$$\lambda(\varepsilon, \varepsilon') = \begin{cases} 1 & \text{if } (\varepsilon, \varepsilon') \text{ is equal to } (1, 0), \\ 2 & \text{if } (\varepsilon, \varepsilon') \text{ is equal to } (0, 0) \text{ or } (1, 1) \\ 3 & \text{if } (\varepsilon, \varepsilon') \text{ is equal to } (0, 1), \end{cases} \tag{27}$$

Further notations

Let $\mathbf{a}$ be a non empty admissible composition. Let $\varepsilon_1 \dots \varepsilon_k$ denote the corresponding binary word $\mathbf{w}(\mathbf{a})$. For any index i such that $1 \leqslant i \leqslant k-1$, let $\mathbf{a}_i$ and $\mathbf{b}_i$ denote the compositions corresponding to the binary words $\varepsilon_{i+1} \dots \varepsilon_k$ and $\overline{\varepsilon_i} \dots \overline{\varepsilon_1}$ respectively

Generalization of Euler's classical formula

Theorem

— *Let* $\mathbf{a}$ *be a non empty admissible composition. Then We have*

$$\zeta(\mathbf{a}) = \sum_{m=1}^{\infty} \psi_m(\mathbf{a}) \binom{2m}{m}^{-1} \tag{28}$$

where for each $m \geqslant 1$

$$\psi_m(\mathbf{a}) = \sum_{i=1}^{k-1} \lambda(\varepsilon_i, \varepsilon_{i+1}) \varphi_m(\mathbf{a}_i) \varphi_m(\mathbf{b}_i). \tag{29}$$

faster than the standard algorithm

It is faster than the first one when one is only interested in computing a single multiple zeta value.

It is also faster than the standard algorithm, based on evaluations of multiple polylogarithms at $\frac{1}{2}$, which has been for example implemented by J. Borwein, P. Lisonek, P. Irvine and C. Chan on their website EZ-Face
http://wayback.cecm.sfu.ca/projects/EZFace/Java/index.html

Generalization of this formula

As Henri Cohen pointed us in a private communication, our algorithms can be extended to compute values of multiple polylogarithms (in many variables). We are most grateful to him for providing us with this possible extension of our work and we hope to address this question in depth in the future.

Implementation Details

This algorithm, implemented in Python 2.7.5 on my personal computer took for example 10.1 seconds to compute $\zeta(2,1,3,2)$ with 1000 exact decimal places and 0.24 seconds with only 100 exact decimal places. Implemented later by Henri Cohen in C it took 0.08 and 0.001 seconds respectively.

Another algorithm previously used to compute $\zeta(\mathbf{a})$, and for example implemented on the site EZ-face quoted in the introduction, is based on the following identity

$$\zeta(\mathbf{a}) = \sum_{i=0}^{k} \mathrm{Li}_{\mathbf{a}_i}(\frac{1}{2})\mathrm{Li}_{\mathbf{b}_i}(\frac{1}{2}) \tag{30}$$

where $\mathbf{a}_i$ and $\mathbf{b}_i$ are defined as before and

$$\mathrm{Li}_{(a_1,\ldots,a_r)}(z) = \sum_{n_1>\ldots>n_r>0} \frac{z^{n_1}}{n_1^{a_1}\ldots n_r^{a_r}}.$$

for any composition $(a_1,\ldots,a_r)$ and any $z \in \mathbf{C}$ such that $|z| < 1$.

our algorithm requires only half as many steps as the old one to achieve the same precision, and implemented on the same computer, it takes roughly a third of the time. Moreover, the old algorithm looks somewhat artificial, because it involves splitting the iterated integral from 0 to 1 at $\frac{1}{2}$, whereas one could also choose any other intermediate element between 0 and 1.

Multiple Apéry-Like Sums