On the algebra of multiple q-Zeta Values

Ulf Kühn - Universität Hamburg

Desy Zeuthen
Theory Seminar, March 2018

joint work with Henrik Bachmann, Nagoya University
arXiv:1708.07464 [math.NT]

Multiple zeta values (MZV)

Definition

For natural numbers $s_1 \geqslant 2, s_2, ..., s_l \geqslant 1$ the sum

$$\zeta(s_1, ..., s_l) = \sum_{n_1 > ... > n_l > 0} \frac{1}{n_1^{s_1} \dots n_l^{s_l}}$$

is called a multiple zeta value (MZV) of weight $s_1 + ... + s_l$ and depth l.

- The rules for the product of infinite sums imply that the product of MZV can be expressed as a linear combination of MZV with the same weight (stuffle product).
- MZV can be expressed as iterated integrals. This gives another way (shuffle product) to express the product of two MZV as a linear combination of MZV.
- These two products give a large number of $\mathbb{Q}$-linear relations (extended double shuffle relations) between MZV. Conjecturally these are all relations between MZV, e.g.

$$\zeta(2,3) + 3\zeta(3,2) + 6\zeta(4,1) \overset{\text{shuffle}}{=} \zeta(2) \cdot \zeta(3) \overset{\text{stuffle}}{=} \zeta(2,3) + \zeta(3,2) + \zeta(5) .$$

Dimension conjectures for $\mathcal{MZ}$

Broadhurst-Kreimer Conjecture

The $\mathbb{Q}$-algebra $\mathcal{MZ}$ of multiple zeta values is a free polynomial algebra, which is graded for the weight and filtered for the depth ("depth drop for even zetas"). Set

$$BK(x,y) = \Big(1 + E(x)y\Big) \frac{1}{1 - O_3(x)y + S(x)y^2 - S(x)y^4}$$

with

$$E(x) = \frac{x^2}{1-x^2} = x^2 + x^4 + x^6 + \ldots \qquad \text{"even zetas"},$$

$$O_3(x) = \frac{x^3}{1-x^2} = x^3 + x^5 + x^7 + \ldots \qquad \text{"odd zetas"},$$

$$S(x) = \frac{x^{12}}{(1-x^4)(1-x^6)} = x^{12} + x^{16} + x^{18} + \ldots \qquad \text{"period polynomials"}.$$

Then the numbers $g_{k,l}$ of generators in weight $k \geqslant 3$ and depth l are determined by

$$BK(x,y) = \sum_{k,l \geqslant 0} \dim_{\mathbb{Q}} \left(\mathrm{gr}^{W,D}_{k,l} \, \mathcal{MZ} \right) x^k y^l = \Big(1 + E(x)\,y\Big) \prod_{k \geqslant 3, l \geqslant 1} \frac{1}{\left(1 - x^k y^l\right)^{g_{k,l}}}$$

Dimension conjectures for $\mathcal{MZ}$

Zagier's Conjecture

The following identities hold:

$$Zag(x) = \sum_{k \geqslant 0} \dim_{\mathbb{Q}} \left(\mathrm{gr}_k^W \, \mathcal{MZ} \right) x^k = \frac{1}{1 - x^2 - x^3}.$$

Zagier's conjecture is implied by Broadhurst-Kreimer's conjecture. In order to neglect the depth we just have to set $y = 1$ and get

$$Zag(x) = BK(x, 1) = \frac{1 + E(x)}{1 - O(x)} = \frac{1 + \frac{x^2}{1-x^2}}{1 - \frac{x^3}{1-x^2}} = \frac{1}{1 - x^2 - x^3}.$$

Brown's Theorem

The $\mathbb{Q}$-vector space of multiple zeta values is spanned by the 23-MZV's, e.g. by those $\zeta(s_1, \ldots, s_l)$ with $s_i \in \{2, 3\}$.

By Brown's theorem the dimensions in Zagier's conjecture are the maximal possible ones.

multiple q-zeta values

Many of the most basic concepts in mathematics have so-called q-analogues, where q is a formal variable such that the specialisation $q = 1$ recovers the usual concept. Attributed to Gauss are the q-integers

$$\{n\}_q = 1 + q + \ldots + q^{n-1} = \frac{1-q^n}{1-q}.$$

We will study the following q-analogues of multiple zeta values.

Definition [(modified) multiple q-zeta-value]

For $s_1, \ldots, s_l \geqslant 1$ and polynomials $Q_1(t) \in t\mathbb{Q}[t]$ and $Q_2(t) \ldots, Q_l(t) \in \mathbb{Q}[t]$ we define

$$\zeta_q(s_1, \ldots, s_l; Q_1, \ldots, Q_l) = \sum_{n_1 > \cdots > n_l > 0} \frac{Q_1(q^{n_1}) \ldots Q_l(q^{n_l})}{(1-q^{n_1})^{s_1} \cdots (1-q^{n_l})^{s_l}} \in \mathbb{Q}[[q]].$$

This series can be seen as a q-analogue of multiple zeta values, since we have for $s_1 > 1$

$$\lim_{q \to 1} (1-q)^{s_1 + \cdots + s_l} \zeta_q(s_1, \ldots, s_l; Q_1, \ldots, Q_l) = Q_1(1) \ldots Q_l(1) \cdot \zeta(s_1, \ldots, s_l).$$

Observe, just replacing n by $\{n\}_q$ in multiple zeta values will not work.

Algebra of multiple q-zeta values

We consider the following $\mathbb{Q}$-algebra:

$$\mathcal{Z}_q := \left\langle \zeta_q(s_1, \ldots, s_l; Q_1, \ldots, Q_l) \;\middle|\; l \geqslant 0,\ s_1, \ldots, s_l \geqslant 1,\ \deg(Q_j) \leqslant s_j \right\rangle_{\mathbb{Q}}.$$

In depth one for example it is

$$\zeta_q(s_1; Q_1) \cdot \zeta_q(s_2; Q_2) = \zeta_q(s_1, s_2; Q_1, Q_2) + \zeta_q(s_2, s_1; Q_2, Q_1) + \zeta_q(s_1 + s_2; Q_1 \cdot Q_2),$$

and clearly $\deg Q_1 \cdot Q_2 \leqslant s_1 + s_2 - d$ if $\deg Q_j \leqslant s_j - d$ for $j = 1, 2$.

Caution, we have for example

$$\zeta_q(s; Q) = \zeta_q(s + 1, (1 - t) \cdot Q(t))$$

thus, contrary to the case of MZVs, the number $s_1 + \cdots + s_l$ does not give a good notion of weight for the ζ_q. Also the number l will not be used to define the depth.

Instead we will consider a class of q-series which also span the space $\mathcal{Z}_q$ and use these series to define a weight and a depth filtration on $\mathcal{Z}_q$.

Bi-brackets

Definition

For $s_1, \dots, s_l \geqslant 1, r_1, \dots, r_l \geqslant 0$ we set $\kappa = \big(r_1!(s_1-1)! \dots r_l!(s_l-1)!\big)^{-1}$ and define

$$\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} := \kappa \cdot \sum_{\substack{u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} u_1^{r_1} \dots u_l^{r_l} \cdot v_1^{s_1-1} \dots v_l^{s_l-1} \cdot q^{u_1 v_1 + \dots + u_l v_l} \in \mathbb{Q}[[q]] \,.$$

We refer to these q-series as *bi-brackets* of depth l and weight $s_1 + \dots + s_l + r_1 + \dots + r_l$.

For $n \in \mathbb{N}$ and natural numbers $r_1, \dots, r_l \geqslant 0$, $s_1, \dots, s_l > 0$ we call

$$\sigma_{\substack{s_1, \dots, s_l \\ r_1, \dots, r_l}}(n) := \sum_{\substack{u_1 v_1 + \dots + u_l v_l = n \\ u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} u_1^{r_1} v_1^{s_1} \dots u_l^{r_l} v_l^{s_l}$$

the bi-multiple divisor sum of n with bi index ${\substack{s_1, \dots, s_l \\ r_1, \dots, r_l}}$. Then their generating series equals

$$\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} = \kappa \cdot \sum_{n>0} \sigma_{\substack{s_1-1, \dots, s_l-1 \\ r_1, \dots, r_l}}(n)\, q^n \,.$$

Multiple divisor sums and modular forms

If $r_1 = \cdots = r_l = 0$, then we write $[s_1, \ldots s_l] = \left[{s_1,\ldots,s_l \atop 0,\ldots,0}\right]$. These are called brackets and we conclude

$$[s_1, \ldots, s_l] = \frac{1}{(s_1-1)!\ldots(s_l-1)!}\sum_{n>0}\sigma_{s_1-1,\ldots,s_l-1}(n)q^n\,.$$

We call the coefficients $\sigma_{s_1-1,\ldots,s_l-1}(n)$ **multiple divisor sums**, they are given by

$$\sigma_{s_1-1,\ldots,s_l-1}(n) := \sum_{\substack{u_1v_1+\cdots+u_lv_l=n\\ u_1>\cdots>u_l>0\\ v_1,\ldots,v_l>0}} v_1^{s_1}\ldots v_l^{s_l}\,.$$

In the case $l = 1$ we get the classical divisor sums $\sigma_{k-1}(n) = \sum_{d|n} d^{k-1}$ and

$$[k] = \frac{1}{(k-1)!}\sum_{n>0}\sigma_{k-1}(n)q^n\,.$$

These function appear in the Fourier expansion of classical Eisenstein series which are (quasi)-modular forms for $SL_2(\mathbb{Z})$, for example

$$G_2 = -\frac{1}{24} + [2]\,, \quad G_4 = \frac{1}{1440} + [4]\,, \quad G_6 = -\frac{1}{60480} + [6]\,.$$

Bi-brackets and Eulerian polynomials

The bi-brackets can also be written as

$$\begin{bmatrix} s_1,\dots,s_l \\ r_1,\dots,r_l \end{bmatrix} = \kappa \cdot \sum_{n_1>\dots>n_l>0} \frac{n_1^{r_1} P_{s_1-1}(q^{n_1}) \dots n_l^{r_l} P_{s_l-1}(q^{n_l})}{(1-q^{n_1})^{s_1} \dots (1-q^{n_l})^{s_l}} \,,$$

where the $P_{k-1}(t)$ are the Eulerian polynomials defined by

$$\frac{P_{k-1}(t)}{(1-t)^k} = \mathrm{Li}_{1-k}(t) = \sum_{d>0} d^{k-1} t^d \,.$$

$$P_0(t) = P_1(t) = t\,, \quad P_2(t) = t^2 + t\,, \quad P_3(t) = t^3 + 4t^2 + t\,,$$

$$\begin{bmatrix} 1,1 \\ 0,1 \end{bmatrix} = \sum_{n_1>n_2>0} \frac{q^{n_1} n_2 q^{n_2}}{(1-q^{n_1})(1-q^{n_2})}\,,$$

$$\begin{bmatrix} 4,2,1 \\ 2,0,5 \end{bmatrix} = \frac{1}{3!\cdot 2!\cdot 5!} \sum_{n_1>n_2>n_3>0} \frac{n_1^2 (q^{3n_1} + 4q^{2n_1} + q^{n_1}) \cdot q^{n_2} \cdot n_3^5 q^{n_3}}{(1-q^{n_1})^4 \cdot (1-q^{n_1})^2 \cdot (1-q^{n_1})^1}\,.$$

Bi-brackets and multiple q-zeta values

Theorem (Bachmann-K.)

The following equalities hold

(i) $$\mathcal{Z}_q = \left\langle \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} \mid l \geqslant 0, s_1, \dots, s_l \geqslant 1, \, r_1, \dots, r_l \geqslant 0 \right\rangle_{\mathbb{Q}} .$$

(ii) $$\mathcal{Z}_q^\circ = \left\langle \zeta_q(s_1, \dots, s_l; Q_1, \dots, Q_l) \in \mathcal{Z}_q \mid Q_2, \dots, Q_l \in t\mathbb{Q}[t] \right\rangle_{\mathbb{Q}}$$
$$= \left\langle [s_1, \dots, s_l] \mid l \geqslant 0 \, , s_1, \dots, s_l \geqslant 1 \right\rangle_{\mathbb{Q}} .$$

Idea of proof:

$$\begin{aligned}
\begin{bmatrix} 1, 1 \\ 0, 1 \end{bmatrix} &= \sum_{n_1 > n_2 > 0} \frac{q^{n_1}}{(1 - q^{n_1})} \frac{n_2 q^{n_2}}{(1 - q^{n_2})} \\
&= \sum_{n_1 > n_2 > 0} \frac{q^{n_1}}{(1 - q^{n_1})} \frac{q^{n_2}}{(1 - q^{n_2})} + \sum_{n_1 > n_2 > n_3 > 0} \frac{q^{n_1}}{(1 - q^{n_1})} \frac{q^{n_2}}{(1 - q^{n_2})} \frac{1 - q^{n_3}}{(1 - q^{n_3})} \\
&= \zeta_q(1, 1; t, t) + \zeta_q(1, 1, 1; t, t, 1 - t) \, .
\end{aligned}$$

Depth- and weight-filtration

We endow the space of multiple q-zeta values $\mathcal{Z}_q$ with the depth- resp. weight-filtration induced by the notion of weight and depth defined on the bi-brackets

bi-brackets - algorithm

Algorithm

There exists a parallel and recursive algorithm that calculates lower bounds to the dimensions of the vector spaces $\mathrm{Fil}^{\mathrm{W,D}}_{k,l}(\mathcal{Z}_q)$. It also applies to the sub-spaces determined bi-brackets of certain kind filtered by the depth and the weight , e.g. $\mathcal{Z}_q^{\circ}$ or "123-brackets".

Main ideas:

The algorithm will calculate a sufficient large number of coefficients, which in turn allows us to prove linear independencies. An approximated version of a bi-brackets is defined as

$$\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix}_N := \sum_{N \geqslant n_1 > \cdots > n_l > 0} \prod_{j=1}^{l} \left(\frac{n_j^{r_j}}{r_j!} \cdot \frac{q^{n_j} P_{s_j-1}(q^{n_j})}{(s_j-1)! \cdot (1-q^{n_j})^{s_j}} \right) \in \mathbb{Q}[[q]].$$

It is clear that at least the first N coefficients of these approximated versions are identical to the bi-brackets, i.e.

$$\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix}_N \equiv \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} \mod q^{N+1}.$$

Lemma (Recursive calculation)

For all $s_1, \ldots, s_l, r_1, \ldots, r_l$ and $N \geqslant l$ we have

$$\begin{bmatrix} s_1, \ldots, s_l \\ r_1, \ldots, r_l \end{bmatrix}_N = \begin{bmatrix} s_1, \ldots, s_l \\ r_1, \ldots, r_l \end{bmatrix}_{N-1} + \frac{N^{r_1}}{r_1!} \frac{q^N P_{s_1-1}(q^N)}{(s_1-1)! \cdot (1-q^N)^{s_1}} \begin{bmatrix} s_2, \ldots, s_l \\ r_2, \ldots, r_l \end{bmatrix}_{N-1},$$

where we set $\begin{bmatrix} s_2, \ldots, s_l \\ r_2, \ldots, r_l \end{bmatrix}_{N-1} = 1$ for $l = 1$.

The algorithm determines at first a set of tree-like lists of weights. Then for each of these lists the Lemma will be applied, i.e. in n-th STEP we obtain lists of the form

$$\left[.., [\begin{bmatrix} s_l \\ r_l \end{bmatrix}_n, 0], .., [\begin{bmatrix} s_{l-1}, s_l \\ r_{l-1}, r_l \end{bmatrix}_n, \mathrm{pos}(\begin{bmatrix} s_l \\ r_l \end{bmatrix}_n)], .., [\begin{bmatrix} s_{l-2}, s_{l-1}, s_l \\ r_{l-2}, r_{l-1}, r_l \end{bmatrix}_n, \mathrm{pos}(\begin{bmatrix} s_{l-1}, s_l \\ r_{l-1}, r_l \end{bmatrix}_n)], ..\right]$$

where $\mathrm{pos}(*)$ points to the position of $*$ in the list. □

We implemented this algorithm in parallel PARI/GP and on a computer with 32 cores /400 GB RAM it takes a night to obtain each of the following tables:

bi-brackets - experiments

$k\backslash l$	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	2	0	0	0	0	0	0	0	0	0	0	0	0	0
2	3	4	0	0	0	0	0	0	0	0	0	0	0	0
3	5	7	8	0	0	0	0	0	0	0	0	0	0	0
4	7	12	14	15	0	0	0	0	0	0	0	0	0	0
5	10	19	25	27	28	0	0	0	0	0	0	0	0	0
6	13	30	41	48	50	51	0	0	0	0	0	0	0	0
7	17	44	68	81	89	91	92	0	0	0	0	0	0	0
8	21	65	106	138	153	162	164	165	0	0	0	0	0	0
9	26	90	167	223	264	281	291	293	294	0	0	0	0	0
10	31	126	249	366	439	490	509	520	522	523	0	0	0	0
11	37	167	376	571	738	830	892	913	925	927	928	0	0	0
12	43	222	537	905	1190	1418	1531	1605	1628	1641	1643	1644	0	0
13	50	285	778	1364	1948	2344	2645	2781	2868	2893	2907	2909	2910	0
14	57	368	1075	2090	3051	3923	4453	4840	5001	5102	5129	5144	5146	5147

Table : lower bounds for $\dim_{\mathbb{Q}} \mathrm{Fil}^{\mathrm{W},\mathrm{D}}_{k,l}(\mathcal{Z}_q)$ with big depth

bi-brackets - experiments

$l\backslash k$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
1	2	3	5	7	10	13	17	21	26	31	37	43	50	57	65	73	82	91	101	111	122
2	0	4	7	12	19	30	44	65	90	126	167	222	285	368	460	577	706	866	1041	1254	1485
3	0	0	8	14	25	41	68	106	167	249	376	537	778	1075	1503	2017	2737	3584	4739	6077	7859

Table : lower bounds for $\dim_{\mathbb{Q}} \mathrm{Fil}_{k,l}^{\mathrm{W,D}}(\mathcal{Z}_q)$ with small depth

We have similar tables for various sub-algebras like $\mathcal{Z}_q^\circ$, $\mathcal{Z}_{q,1}^\circ$ or subsets like the "123-brackets". By setting

$$\mathrm{gr}_{k,l}^{\exp}(\mathcal{Z}_q) = \mathrm{fil}_{k,l}^{W,L}(\mathcal{Z}_q) - \mathrm{fil}_{k,l-1}^{W,L}(\mathcal{Z}_q) - \mathrm{fil}_{k-1,l}^{W,L}(\mathcal{Z}_q) + \mathrm{fil}_{k-1,l-1}^{W,L}(\mathcal{Z}_q)$$

we get then the tables we study for pattern.

bi-brackets - experiments

$\mathrm{gr}^{\exp}_{k\backslash l}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	1	0	0	0	0	0	0	0	0	0	0	0	0
3	2	1	1	0	0	0	0	0	0	0	0	0	0	0
4	2	3	1	1	0	0	0	0	0	0	0	0	0	0
5	3	4	4	1	1	0	0	0	0	0	0	0	0	0
6	3	8	5	5	1	1	0	0	0	0	0	0	0	0
7	4	10	13	6	6	1	1	0	0	0	0	0	0	0
8	4	17	17	19	7	7	1	1	0	0	0	0	0	0
9	5	20	36	24	26	8	8	1	1	0	0	0	0	0
10	5	31	46	61	32	34	9	9	1	1	0	0	0	0
11	6	35	86	78	94	41	43	10	10	1	1	0	0	0
12	6	49	106	173	118	136	51	53	11	11	1	1	0	0
13	7	56	178	218	299	168	188	62	64	12	12	1	1	0
14	7	76	214	429	377	476	229	251	74	76	13	13	1	1

$g^{\exp}_{k\backslash l}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	2	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	1	0	0	0	0	0	0	0	0	0	0	0	0
5	3	0	1	0	0	0	0	0	0	0	0	0	0	0
6	0	2	0	1	0	0	0	0	0	0	0	0	0	0
7	4	0	3	0	1	0	0	0	0	0	0	0	0	0
8	0	7	0	3	0	1	0	0	0	0	0	0	0	0
9	5	0	8	0	4	0	1	0	0	0	0	0	0	0
10	0	12	0	11	0	4	0	1	0	0	0	0	0	0
11	6	0	22	0	14	0	5	0	1	0	0	0	0	0
12	0	20	0	31	0	17	0	5	0	1	0	0	0	0
13	7	0	47	0	44	0	21	0	6	0	1	0	0	0
14	0	31	0	81	0	58	0	25	0	6	0	1	0	0

Table : $\sum_{k,l} \mathrm{gr}^{\exp}_{k,l}(\mathcal{Z}_q)\, x^k y^l = \chi_{\widetilde{M}}(x,y) \cdot \prod_{k,l \geqslant 0} \frac{1}{(1-x^k y^l)^{g^{\exp}_{k,l}}}$

with

$$\chi_{\widetilde{M}}(x,y) = \sum_{k,l \geqslant 0} \mathrm{gr}_{k,l}(\widetilde{M}(\mathrm{SL}_2(\mathbb{Z}))\, x^k y^l$$

$$= 1 + \frac{x^2}{(1-x^2)^2}\, y + \frac{x^{12}}{(1-x^2)(1-x^4)(1-x^6)}\, y^2 .$$

bi-brackets - experiments

$gr^{\exp}_{k\backslash l}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
3	1	2	1	0	0	0	0	0	0	0	0	0	0	0	0
4	0	3	3	1	0	0	0	0	0	0	0	0	0	0	0
5	0	2	6	4	1	0	0	0	0	0	0	0	0	0	0
6	0	1	7	9	5	1	0	0	0	0	0	0	0	0	0
7	0	0	6	15	13	6	1	0	0	0	0	0	0	0	0
8	0	0	3	19	25	18	7	1	0	0	0	0	0	0	0
9	0	0	1	16	40	39	24	8	1	0	0	0	0	0	0
10	0	0	0	10	50	70	58	31	9	1	0	0	0	0	0
11	0	0	0	4	45	108	115	83	39	10	1	0	0	0	0
12	0	0	0	1	30	131	199	180	115	48	11	1	0	0	0
13	0	0	0	0	15	126	287	341	271	155	58	12	1	0	0
14	0	0	0	0	5	90	351	554	555	395	204	69	13	1	0
15	0	0	0	0	1	50	351	774	990	868	560	263	81	14	1

$a^{\exp}_{k\backslash l}$	1	2	3	4	5	6	7	8	9	10
1	-1	0	0	0	0	0	0	0	0	0
2	-1	0	0	0	0	0	0	0	0	0
3	-1	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0
6	0	0	0	1	0	0	0	0	0	0
7	0	0	0	1	0	0	0	0	0	0
8	0	0	0	0	1	0	0	0	0	0
9	0	0	0	0	1	0	0	0	0	0
10	0	0	0	0	-1	1	0	0	0	0
11	0	0	0	0	0	1	-1	0	0	0
12	0	0	0	0	0	1	-1	0	0	0
13	0	0	0	0	0	-1	3	-2	0	0
14	0	0	0	0	0	0	4	-4	0	0
15	0	0	0	0	0	0	-7	9	-2	0

Table : $\sum_{k,l\geqslant 0} \mathrm{gr}^{\exp}_{k,l}(\text{"123-brackets"})\, x^k y^l = \frac{1}{1+\sum_{k,l\geqslant 0} a^{\exp}_{k,l} x^k y^l}$

bi-brackets - conjectures

Conjectures w.r.t. the algebra structures

(S1) The algebra $\mathcal{Z}_q$ is isomorphic to a free polynomial algebra.

(S2) We have a decomposition of $\mathbb{Q}$-algebras

$$\mathcal{Z}_q \cong \widetilde{M}_{\mathbb{Q}}(SL_2(\mathbb{Z})) \otimes \mathcal{A},$$

moreover $\mathcal{A}$ equals the graded dual of the universal enveloping algebra of a bi-graded Lie-algebra.

Conjectures w.r.t. the vector space basis

(B1) Every bi-bracket equals a linear combination of brackets, i.e. $\mathcal{Z}_q^\circ = \mathcal{Z}_q$.

(B2) Every bi-bracket equals a linear combination of 123-brackets.

Conjectures w.r.t. the graded dimensions

(D1) We have

$$\sum_{k \geqslant 0} \dim_{\mathbb{Q}} \mathrm{gr}_k^{\mathrm{W}}(\mathcal{Z}_q) x^k = \frac{1}{1 - x - x^2 - x^3 + x^6 + x^7 + x^8 + x^9}.$$

Conjectures w.r.t. the graded dimensions

(D2) We have

$$\sum_{w,l\geqslant 0} \dim \mathrm{gr}^{\mathrm{W,D}}_{k,l}(\mathcal{Z}_q)\, x^k y^l = \chi_{\widetilde{M}}(x,y) \,\cdot\, \chi_{\mathcal{A}}(x,y),$$

with

$$\chi_{\mathcal{A}}(x,y) = 1/\Big(1 - a_1(x)\, y + a_2(x)\, y^2 - a_3(x)\, y^3 - a_4(x)\, y^4 + a_5(x)\, y^5\Big),$$

$$\begin{aligned} a_1(x) &= D(x)\, O_1(x) \\ a_2(x) &= D(x) \sum_{k\geqslant 4} \dim(M_k(\mathrm{SL}_2(\mathbb{Z}))^2\, x^k \\ a_3(x) &= O_1(x)\, S(x) = a_5(x) \\ a_4(x) &= D(x) \sum_{k\geqslant 12} \dim(S_k(\mathrm{SL}_2(\mathbb{Z}))^2\, x^k \end{aligned}$$

With $D(x) = 1/(1-x^2)$, $O_1(x) = x/(1-x^2)$, $S(x) = x^{12}/((1-x^4)(1-x^6))$ and

$$\chi_{\widetilde{M}}(x,y) = 1 + \frac{x^2}{(1-x^2)^2}\, y + \frac{x^{12}}{(1-x^2)(1-x^4)(1-x^6)}\, y^2.$$

bi-brackets - evidences for the conjectures

If we assume that the lower bounds obtained by the numerical calculations equal the actual dimensions, then the conjectures hold within the range of our experiments.

Theorem (Bachmann-K.)

The conjectures (B1), (B2) and (D1) hold for all weights $k \leqslant 7$, i.e. every bi-bracket is a linear combination of 123-brackets and there are exactly as many linear independent as expected.

Idea of Proof: Via the partition-shuffle-spaces

$$\mathbb{PS}(k-l,l) = \{f \in \mathbb{Q}[x_1,..,x_l,y_1,..,y_l] \,|\, \deg f = k-l,\ f\big|_P - f = f\big|_{\mathrm{Sh}_j} = 0\ \forall j\},$$

with functional equations similar to double shuffle spaces for multiple zeta values, we get the upper bounds for the number $g_{k,l}$ of generators of weight k and depth l for $\mathcal{Z}_q$

$$g_{k,l} \leqslant \dim_{\mathbb{Q}} \mathbb{PS}(k-l,l).$$

Now computing sufficiently many coefficients of the bi-brackets in question gives us lower bounds for $\dim_{\mathbb{Q}} \mathrm{Fil}_k^{\mathrm{W}}(\mathcal{Z}_q)$. Happily both numbers coincide for $k \leqslant 7$.

q-MZV's and Lie-Algebras

The dual of the vector space spanned by the generators for the algebra of (formal) multiple zeta values has the structure of a Lie-algebra $\mathfrak{ds}$ (Ihara, Furusho, Racinet, Goncharov, Brown, ...) and its Lie-bracket is related to Goncharov's coproduct. This Lie algebra $\mathfrak{ds}$ and its refinement $\mathfrak{ls}$ can be identified with Lie algebras of "al/al", resp. "al/il", polynomial moulds defined by Ecalle.

So far we have not discovered a coproduct on $\mathcal{Z}_q$, but there are Lie algebras $\mathfrak{zq}$ and $\mathfrak{lzq}$, defined within Ecalle's theory of moulds, that very likely correspond in the above sense to $\mathcal{Z}_q$.

$\mathcal{Z}_q$ and the partition shuffle Lie-Algebra

The partition shuffle Lie-Algebra is a graded Lie-Algebra $\mathfrak{zq} = \bigoplus_{k \geqslant 0} \mathfrak{zq}_k$ with graded pieces

$$\mathfrak{zq}_k = \Big\{ \big(f_1(x_1, y_1),\ f_2(x_1, y_1, x_2, y_2), \dots\big) \,\Big|\, f_i \in \mathbb{Q}[x_1, y_1, \dots, x_i, y_i] \text{\& conditions} \Big\}$$

In particular, if $f_i \neq 0$, then $\deg(f_i) + i = k - 1$, and the f_i satisfy an invariance ("swap-invariant") and some recursive compatibilities ("alternility"). For example we have in degrees 3 and 5

$$\begin{aligned}
\widehat{\xi}_{1,0} &= (1, 0, \dots), \\
\widehat{\xi}_{3,0} &= (x_1^2 + y_1^2,\ x_1 - 2x_2 - y_1 + y_2, \tfrac{1}{3}, 0, \dots), \\
\widehat{\xi}_{2,1} &= (x_1 y_1, -2x_1 + 2x_2 - 2y_2, 0, \dots.), \\
\widehat{\xi}_{5,0} &= (x_1^4 + y_1^4, \dots), \\
\widehat{\xi}_{4,1} &= (x_1 y_1 (x_1^2 + y_1^2), \dots), \\
\widehat{\xi}_{3,2} &= ((x_1 y_1)^2, \dots).
\end{aligned}$$

The Lie-bracket is essentially given by means of Ecalle's ARI-Lie-bracket $\{\ ,\ \}_{ARI}$, i.e. $\{\alpha, \beta\} = \phi^{-1}\{\phi(\alpha), \phi(\beta)\}_{ARI}$, where ϕ maps an alternil to an alternal mould.

Conjecture

The partition shuffle Lie-algebra $\mathfrak{zq}$ is generated by the $\widehat{\xi}_{r,s}$ and quadratic relations generate the ideal of relations. The Hilbert-Poincare series equals

$$H_{\mathcal{U}(\mathfrak{zq})}(x) = \frac{1}{1 - D(x)O_1(x) + D(x)R(x)},$$

where $D(x) = 1/(1-x^2)$, $O_1(x) = x/(1-x^2)$ and $R(x) = \sum_{k \geqslant 4} \dim(S_k \oplus M_k)x^k$.

For example the relation $\{\widehat{\xi}_{1,0}, \widehat{\xi}_{2i+1,0}\} = 0$ for all $i \geqslant 1$ gives the "Eisenstein-part".

Interpretation

If the missing link from $\mathcal{Z}_q$ to $\mathfrak{zq}$ is filled, then the dimension conjecture D1 would be implied, i.e. $\mathcal{Z}_q \cong \widetilde{M}(SL_2(\mathbb{Z})) \otimes \mathcal{U}(\mathfrak{zq})^{\vee}$.

At the level of Hilbert-Poincare series, the above isomorphism is nothing else than the identity

$$\frac{1}{1-x-x^2-x^3+x^6+x^7+x^8+x^9} = \frac{1}{(1-x^2)(1-x^4)(1-x^6)} \frac{1}{1-D(x)O_1(x)+D(x)R(x)}.$$

$\mathcal{Z}_q$ and the linearised partition shuffle Lie-Algebra

The linearised partition shuffle Lie-Algebra $\mathfrak{lzq}$ is a bi-graded Lie-Algebra $\mathfrak{lzq} = \bigoplus_{k,l \geqslant 0} \mathfrak{lzq}_{k,l}$ with graded pieces

$$\mathfrak{lzq}_{k,l} = \left\{ f(x_1, y_1, \ldots, x_l, y_l) \in \mathbb{Q}[x_1, y_1, \ldots, x_l, y_l] \,\middle|\, \deg(f) + l = k \text{ \& conditions} \right\}$$

where the f satisfy a set of many terms functional equations ("alternality") and an invariance ("swap invariance"). The Lie-bracket is given by Ecalle's ARI-Lie-bracket $\{\ ,\ \}_{ARI}$.

Proposition

The map $\mathfrak{zq}_k \longrightarrow \mathfrak{lzq}_{k,l}$ given by

$$(\underbrace{0, \ldots, 0}_{\#=l-1}, \underbrace{f_l(x_1, y_1, \ldots, x_l, y_l), *, \ldots, *}_{\text{"compatibles"}}, 0, \ldots) \mapsto f_l$$

induces an isomorphism $\mathfrak{zq} \cong \mathfrak{lzq}$ of graded Lie algebras.

Using the quadratic relations we obtain this way "new" generators in depth 4, e.g.,

$$\{\widehat{\xi}_{3,0}, \widehat{\xi}_{9,0}\} - 3\,\{\widehat{\xi}_{5,0}, \widehat{\xi}_{7,0}\} = (0, 0, 0, \chi_{\triangle}, *, \ldots).$$

Meta-Conjecture

(i) The $\mathbb{Q}$-algebra $\mathcal{Z}_q$ is a free polynomial algebra and there is an isomorphism

$$\mathcal{Z}_q \cong \widetilde{M}_{\mathbb{Q}}(SL_2(\mathbb{Z})) \otimes \mathcal{A},$$

where $\mathcal{A}$ is isomorphic to the symmetric algebra[a] of the Lie-algebra $\mathfrak{lzq}$.

(ii) There is a Lie-algebra monomorphism $\iota : \mathfrak{ls} \hookrightarrow \mathfrak{lzq}$.

(iii) The Lie-algebra $\mathfrak{lzq}$ is generated by sub-Lie-algebras $\mathfrak{E}$ ("bi-ekmas") and $\mathfrak{C}$ ("bi-carmas").

(iv) The Lie-algebra $\mathfrak{E}$ is generated in depth 1 and contains the images $\iota(\xi_{2i+1})$ of the ekma moulds. Its relations are generated in depth 2 and their number is related to the square of the dimensions of the space of modular forms for $SL_2(\mathbb{Z})$. There are relations in the relations in depth 3 and no other higher homology.

(v) The Lie-algebra $\mathfrak{C}$ is generated in depth 4 and contains the images $\iota(\chi_p)$ of the carma moulds. The Lie-algebra $\mathfrak{C}$ is free.

(vi) The relations in depth 5 coming from $\{\delta^s \iota(\{\xi_1, \chi_p\})\}_{s\in\mathbb{N}}$ together with the relations in depth 2 satisfied by $\mathfrak{F}$ generate all relations of $\mathfrak{lzq}$.

(vii) The free polynomial algebra $\mathcal{A}$ has the Hilbert-Poincare series as in the conjectured graded dimension formula for $\mathcal{Z}_q$.

[a] i.e. the graded dual of the universal enveloping algebra

The Meta-Conjecture is compatible with the dimension conjecture

$$\sum_{k,l\geqslant 0} \dim \mathrm{gr}^{\mathrm{W,D}}_{k,l}(\mathcal{A})\, x^k y^l = \frac{1}{1-a_1(x)\,y+a_2(x)\,y^2-a_3(x)\,y^3-a_4(x)\,y^4+a_5(x)\,y^5},$$

with

$$a_1(x) = D(x)\,O_1(x) \qquad \text{"}\mathfrak{E}\text{-Generators"}$$

$$a_2(x) = D(x) \sum_{k\geqslant 4} \dim(M_k(\mathrm{SL}_2(\mathbb{Z}))^2\, x^k \qquad \text{"}\mathfrak{E}\text{-relations"}$$

$$a_3(x) = O_1(x)\,S(x) \qquad \text{"}\mathfrak{E}\text{-homology"}$$

$$a_4(x) = D(x) \sum_{k\geqslant 12} \dim(S_k(\mathrm{SL}_2(\mathbb{Z}))^2\, x^k \qquad \text{"}\mathfrak{E}\text{-Generators"}$$

$$a_5(x) = O_1(x)\,S(x) \qquad \text{"}\xi_1\text{-orthogonality to carma"}$$

Some of the statements in the Meta-conjecture are actually proven, e.g.

Theorem

The dimension of the vector spaces $\mathfrak{R}_k$ spanned by the relations in weight k and depth 2 for the Lie algebra $\mathfrak{lzq}$ have the generating series

$$\sum_{k\geqslant 4} \dim \mathfrak{R}_k x^k = D(x) \sum_{n\geqslant 4} \dim(M_n(\mathrm{SL}_2(\mathbb{Z}))^2\, x^n, \qquad \left(D(x) = \frac{1}{1-x^2} \right).$$

Idea of proof.

Explicitly these spaces are given by

$$\mathfrak{R}_k = \Big\{ P \in \mathbb{Q}[u_1,u_2,v_1,v_2] \,\Big|\, \text{homogenous, } \deg P = k-2, \text{ such that}$$
$$P\binom{u_1,u_2}{v_1,v_2} + P\binom{u_1+u_2,u_1}{v_2,v_1-v_2} + P\binom{u_2,u_1+u_2}{v_2-v_1,v_1} = 0,$$
$$P\binom{u_1,u_2}{v_1,v_2} + P\binom{u_2,u_1}{v_2,v_1} = 0, \quad P\binom{u_1,u_2}{v_1,v_2} = P\binom{\epsilon u_1,\mu u_2}{\epsilon v_1,\mu v_2}, (\epsilon,\mu \in \{\pm 1\}),$$
$$P\binom{u_1,u_2}{v_1,v_2} = P\binom{v_1,u_2}{u_1,v_2}, \quad P\binom{u_1,u_2}{v_1,v_2} = P\binom{u_1,v_2}{v_1,u_2} \quad \Big\}$$

Following an idea of Zagier we can recover tensorproducts of period polynomials in the subspace spanned by Δ-harmonic solutions of these functional equation.

Experiments using Pari/GP with parallel algorithms give strong support for the conjectures,e.g.

$l\backslash k$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27
1	1	0	2	0	3	0	4	0	5	0	6	0	7	0	8	0	9	0	10	0	11	0	12	0	13	0	14
2	0	0	0	1	0	2	0	7	0	12	0	20	0	31	0	47	0	63	0	89	0	115	0	148	0	186	0
3	0	0	0	0	1	0	3	0	8	0	22	0	47	0	89	0	161	0	270	0	430	0	663	0	983	0	1414
4	0	0	0	0	0	1	0	3	0	11	0	30	0	80	0	182	0	392	0	764	0	1427	0	2507	0	4246	0
5	0	0	0	0	0	0	1	0	4	0	14	0	44	0	124	0	324	0	780	0	1746	0	3666	0	7285	0	13797
6	0	0	0	0	0	0	0	1	0	4	0	17	0	58	0	184	0	519	0	1386	0	3417	0	7969	0	17509	0

Table : dimension of $\mathrm{gr}^{\mathrm{W},\mathrm{D}}_{k,l}\,\mathfrak{C}$, computed / conjectured

Also we calculated in weight 4 the dimension of the graded pieces of $\mathfrak{C}$ spanned by the bi-carmas for weight $k \leqslant 26$. For this we used a Computer at DESY Hamburg with 128 cores and a Terrabyte Ram. For $k = 26$ the calculation took about a week in particular the final step took 393444 seconds $\approx\ 4.5$ days:

```
time:  393444 sec:  CARMA-DIMENSION = 10 for weight = 26 and prime = 71
```

summary

- The $\mathbb{Q}$-algebra of multiple q-zeta values $\mathcal{Z}_q$ is spanned by bi-brackets, i.e., q-series whose coefficients are rational numbers given by sums over partitions. It contains all quasi-modular forms.
- The elements in $\mathcal{Z}_q$ have a direct connection to multiple zeta values.
- There are conjectural formulas for the dimensions $\dim \mathrm{gr}_{k,l}^{\mathrm{W},\mathrm{D}} \mathcal{Z}_q$ and other subspaces.
- Conjecturally every element in $\mathcal{Z}_q$ can be written as a linear combination of 123-brackets. In particular $\mathcal{Z}_q^\circ = \mathcal{Z}_q$.
- The functional equations satisfied by the generating series of bi-brackets modulo products and lower depth give rise to a subspace in the Lie-algebra of bimoulds.
- Conjecturally the generators of $\mathcal{Z}_q$ give a basis of a Lie-algebra contained in the Lie-algebra of swap-invariant, alternal, polynomial bimoulds.
- Massive computer calculations give striking evidence for those conjectures.

MZV's and the double shuffle Lie-Algebra

The double shuffle Lie-Algebra is a graded Lie-Algebra $\mathfrak{ds} = \bigoplus_{k \geqslant 0} \mathfrak{ds}_k$ with graded pieces

$$\mathfrak{ds}_k = \Big\{ \big(f_1(x_1),\ f_2(x_1,x_2),\ f_3(x_1,x_2,x_3), \ldots \big) \Big| f_i \in \mathbb{Q}[x_1, \ldots x_i] \& \text{ conditions} \Big\}$$

In particular, if $f_i \neq 0$, then $\deg(f_i) + i = k - 1$, and the f_i satisfy some many terms functional equations ("alternality") and some recursive compatibilities ("alternility"). For example we have in degrees 3 and 5

$$\widehat{\xi}_3 = (x_1^2,\ x_1 - 2x_2, \tfrac{1}{3}, 0, \ldots),$$

$$\widehat{\xi}_5 = (x_1^4, 2x_1^3 - \tfrac{11}{2} x_1^2 x_2 + \tfrac{9}{2} x_1 x_2^2 - 3x_2^3, 2x_1^2 - \tfrac{11}{2} x_1 x_2 + \tfrac{9}{2} x_1 x_3 - \tfrac{1}{2} x_2^2 + 2x_2 x_3 - \tfrac{1}{2} x_3^2, *, *, 0, \ldots).$$

Conjecture [Ihara-Deligne, Ecalle]

The double shuffle Lie-Algebra is a free Lie-Algebra that is generated by the $\widehat{\xi}_{2i+1} = (x_1^{2i}, \ldots)$

Corollary

The formal multiple zeta values satisfy the Zagier conjecture, i.e. $\mathcal{MZ}^f \cong \mathbb{Q}[\zeta(2)] \otimes \mathcal{U}(\mathfrak{ds})$ and $\sum_{k \geqslant 0} \dim_{\mathbb{Q}}(\mathcal{MZ}_k^f) x^k = \frac{1}{1-x^2-x^3} = \frac{1}{1-x^2} \frac{1}{1-x^3-x^5-x^7-x^9-\ldots}$.

MZV's and the linearised double shuffle Lie-Algebras I

The linearised double shuffle Lie-Algebra is a bi-graded Lie-Algebra $\mathfrak{ls} = \bigoplus_{k,l \geqslant 0} \mathfrak{ds}_{k,l}$ with graded pieces

$$\mathfrak{ls}_{k,l} = \left\{ f(x_1, ..., x_l) \in \mathbb{Q}[x_1, ..., x_l] \,\middle|\, \deg(f) + l = k \,\&\, \text{conditions} \right\}$$

where the f satisfy two sets many terms functional equations ("alternality", "swapped alternality").

Theorem [Ecalle,...]

The map $\mathfrak{ds}_k \longrightarrow \mathfrak{ls}_{k,l}$ given by

$$(\underbrace{0, ..., 0}_{\#=l-1}, \underbrace{f_l(x_1, ..., x_l), *, ..., *}_{\text{"compatibles"}}, 0, ...) \mapsto f_l$$

induces an isomorphism $\mathfrak{ds} \cong \mathfrak{ls}$ of graded Lie algebras.

Period polynomials yield quadratic relations, which in turn gives "new" generators in depth 4, e.g.,

$$\{\widehat{\xi}_3, \widehat{\xi}_9\} - 3\,\{\widehat{\xi}_5, \widehat{\xi}_7\} = (0, 0, 0, \chi_{\triangle}, *, ...).$$

MZV's and the linearised double shuffle Lie-Algebras II

Conjecture [Ecalle, Brown]

The generators of $\mathfrak{ls}$ are the $\xi_{2i+1} = x_1^{2i}$ in depth 1 and the χ_p in depth 4, each depending on a period polynomials p. The ideal of relations is generated in depth 2 and each of its generator depends also on p. Moreover, the Hilbert-Poincare series equals

$$H_{\mathcal{U}(\mathfrak{ls})}(x,y) = \frac{1}{1 - O_3(x)y + S(x)y^2 - S(x)y^4},$$

with

$$O_3(x) = x^3 + x^5 + x^7 + \ldots \qquad \text{"odd zetas"},$$
$$S(x) = x^{12} + x^{16} + x^{18} + \ldots \qquad \text{"period polynomials"}.$$

Corollary

The formal multiple zeta values satisfy the Broadhurst-Kreimer conjecture, i.e. $\mathcal{MZ}^f \cong \mathbb{Q}[\zeta(2)] \otimes \mathcal{U}(\mathfrak{ls})^{\vee}$ and in particular

$$\sum_{k,l \geqslant 0} \dim_{\mathbb{Q}} \left(\mathrm{gr}_{k,l}^{W,D} \mathcal{MZ}^f \right) x^k y^l = BK(x,y).$$

Moulds

Let A be an alphabet and denote by A^* its words. A Mould $M^\bullet$ is a map from A^* to a Ring R. Observe there is a bijection between moulds and non-commutative power series

$$\{M^\bullet : A^* \to R\} \cong R\langle\langle A \rangle\rangle,$$

since the coefficients of $\sum_{a \in A^*} M^{\underline{a}} a \in R\langle\langle A \rangle\rangle$ determine a mould M uniquely.

Proposition

The set of moulds with values in a ring R is a ring with addition and multiplication given by

$$(A+B)^{a_{i_1} a_{i_2} \cdots a_{i_l}} = A^{a_{i_1} a_{i_2} \cdots a_{i_l}} + B^{a_{i_1} a_{i_2} \cdots a_{i_l}},$$

$$(A \cdot B)^{a_{i_1} a_{i_2} \cdots a_{i_l}} = \sum_{j=0}^{l} A^{a_{i_1} \cdots a_{i_j}} B^{a_{i_j} \cdots a_{i_l}}.$$

Example 1

Let $A = \{a_1, a_2, a_3, ...\}$ be a countable alphabet and let $R = k[[x_1, x_2, x_3, ...]]$ be the ring of formal power series with coefficients in a ring k in a countable number of variables. Then a sequence $f_0 \in k \subset R$, $f_1(x_1) \in k[[x_1]] \subset R$, $f_2(x_1, x_2) \in k[[x_1, x_2]] \subset R$, $f_3(x_1, x_2, x_3) \in k[[x_1, x_2, x_3]] \subset R$, ... of elements in R with a increasing number of variables let us allow to define a mould via

$$\begin{aligned} M^\bullet : \ A^* &\to R \\ a_{i_1} a_{i_2} ... a_{i_l} &\mapsto f_l(x_{i_1}, x_{i_2}, ..., x_{i_l}), \end{aligned}$$

here $f_l(x_{i_1}, x_{i_2}, ..., x_{i_l}) \in k[[x_{i_1}, x_{i_2}, ..., x_{i_l}]] \subset R$ is obtained by applying the obvious coordinate changes $x_j \to x_{i_j}$ to f_l.

By abuse of notation we just write $M(x_{i_1}, x_{i_2}, ..., x_{i_l})$ instead of $M^{a_{i_1} a_{i_2} \cdots a_{i_l}}$. Thus, the example explains the meaning of Ecalle's definition:

A mould is a collection of functions depending on a variable number of variables

Polynomial moulds

Let A be an alphabet. A mould

$$M^\bullet : A^* \to k[x_1, x_2, x_3, ...]$$

is called a polynomial mould.
A particular case is given by a sequence $\{f_i\}_{i\in\mathbb{N}}$ with

$$f_i = \begin{cases} f_l(x_1, ..., x_l) \in k[x_1, x_2, ..., x_l] & \text{if } i = l \\ 0 \in k[x_1, x_2, x_3, ...] & \text{if } i \neq l, \end{cases}$$

then as in Example 1 we get a polynomial mould $M : A^* \to k[x_1, x_2, x_3, ...]$ via

$$M^{\underline{a}} = \begin{cases} f_l(x_{i_1}, x_{i_2}, ..., x_{i_l}) & \text{if } \underline{a} = a_{i_1} a_{i_2} ... a_{i_l} \\ 0 & \text{else.} \end{cases}$$

Properties of Moulds

Key remark

Most properties assigned to moulds correspond to symmetric many term functional equations.

Example: The mould $M^{\bullet} : A \to k(x_1, x_2, x_3, \ldots)$ given by $M^{\underline{a}} = 0$ if the word $\underline{a}$ is empty, has only one letter or if $\underline{a}$ has a repeated letter and for all other cases via the sequence

$$f_l(x_1, \ldots, x_l) = \frac{1}{x_2 - x_1} \frac{1}{x_3 - x_2} \cdots \frac{1}{x_l - x_{l-1}} \in k(x_1, \ldots, x_l)$$

is alternal, i.e.

$$\sum_{\underline{b} \in \mathrm{sh}(\underline{a}_1, \underline{a}_2)} M^{\underline{b}} = 0.$$

In particular for $l = 2, 3, 4$ we have
$M(x_1, x_2) + M(x_2, x_1) = 0,$
$M(x_1, x_2, x_3) + M(x_2, x_1, x_3) + M(x_2, x_3, x_1) = 0,$
$M(x_1, x_2, x_3, x_4) + M(x_2, x_1, x_3, x_4) + M(x_2, x_3, x_1, x_4) + M(x_2, x_3, x_4, x_1) = 0,$
$M(x_1, x_2, x_3, x_4) + M(x_1, x_3, x_2, x_4) + M(x_1, x_3, x_4, x_2) + M(x_3, x_1, x_2, x_4) +$
$M(x_3, x_1, x_4, x_2) + M(x_3, x_4, x_1, x_2) = 0.$

Bimoulds

Let $A = \{w_1, w_2, ...\}$. A mould

$$M^\bullet : A^* \to R = k[[u_1, v_1, u_2, v_2, u_3, v_3, ...]]$$

made with a sequence $f_0 \in k$, $f_1 \in k[[u_1, v_1]]$ and $f_l \in k[[u_1, v_1, u_2, v_2, ..., u_l, v_l]]$ for all $l \geqslant 2$ will be called a bimould in the variables u_i and v_i. We will use the notation

$$M\binom{u_1,u_2,\dots,u_l}{v_1,v_2,\dots,v_l} = M^{a_{i_1}a_{i_2}\dots a_{i_l}} = f_l(u_{i_1}, v_{i_1}, ..., u_{i_l}, v_{i_l}).$$

Sometimes the identification $\underline{w} = \binom{\underline{u}}{\underline{v}}$ is used.

A bimould $M\binom{\underline{u}}{\underline{v}}$ is alternal if M is alternal w.r.t. to both variables simultanously.

Any mould $M(\underline{u})$ as in Example 1 becomes a bimould by setting $M\binom{\underline{u}}{\underline{v}} = M(\underline{u})$

There are symmetries of moulds $M^\bullet : A^* \to R$ induced by endomorphisms of R. The involution *swap* is of particular interest for us

$$\mathrm{swap}(M\binom{u_1,u_2,\dots,u_l}{v_1,v_2,\dots,v_l}) = M\binom{v_l,v_{l-1}-v_l,\dots,v_1-v_2}{u_1+\dots+u_l,u_1+\dots+u_{l-1},\dots,u_1}$$

A mould M is bi-alternal if $M(\underline{u})$ and $M^\sharp(\underline{v}) = \mathrm{swap}(M(\underline{u}))$ are alternal.

ARI Lie-bracket

Decompose a bi-word $w = \binom{u_1,\dots,u_l}{v_1,\dots,v_l}$ into $w = abc$ with

$$a = \binom{u_1,\dots,u_r}{v_1,\dots,v_r}, \quad b = \binom{u_{r+1},\dots,u_{r+s}}{v_{r+1},\dots,v_{r+s}}, \quad c = \binom{u_{r+s+1},\dots,u_l}{v_{r+s+1},\dots,v_l}.$$

then their flexions are defined by $\lceil c = c$ and $a\rceil = a$ if $b = \emptyset$, $b\rfloor = b$ if $c = \emptyset$, $\lfloor b = b$ if $a = \emptyset$ and else by

$$b\rfloor = \binom{u_{r+1},\dots,u_{r+s}}{v_{r+1}-v_{r+s+1},\dots,v_{r+s}-v_{r+s+1}}, \quad \lceil c = \binom{u_{r+1}+\dots+u_{r+s+1},u_{r+s+2},\dots,u_l}{v_{r+s+1},v_{r+s+2}\dots,v_l}$$

$$a\rceil = \binom{u_1,\dots,u_{r-1},u_r+u_{r+1}+\dots+u_{r+s}}{v_1,\dots,v_{r-1},v_r}, \quad \lfloor b = \binom{u_{r+1},\dots,u_{r+s}}{v_{r+1}-v_r,\dots,v_{r+s}-v_r}$$

Definition

The Ari Lie-bracket of two bimoulds is defined with above notation as

$$ari(A,B)(w) = \sum_{\substack{w=abc\\ b\neq\emptyset}} A(a\lceil c)B(b\rfloor) - B(a\lceil c)A(b\rfloor) - \sum_{\substack{w=abc\\ a,b\neq\emptyset}} A(a\rceil c)B(\lfloor b) - B(a\rceil c)A(\lfloor b).$$

ARI Lie-bracket

Theorem (Ecalle, Schneps)

(i) The set of bimoulds $Bari$ equipped with the Ari Lie-bracket is a Lie Algebra.
(ii) The subset $Ari^{pol}_{\underline{al},\underline{al}} \subset Bari$ of bi-alternal polynomial moulds which are even in depth $l = 1$ is a sub Lie algebra.
(iii) The subset $Bari^{pol}_{\underline{al},swap} \subset Bari$ of alternal, swap invariant, neg-invariant bimoulds which are even in depth $l = 1$ is a sub Lie algebra.

By a theorem of Racinet we know that the Lie sub algebra $Ari^{pol}_{\underline{al},\underline{al}}$ is isomorphic to a sub Lie algebra of the free algebra on two generators equipped with the Poisson or equivalently the Ihara Lie bracket.

Proposition

The the linear span of the double shuffle spaces

$$\mathbb{DS}(k-l,l) = \{f \in \mathbb{Q}[x_1,...,x_l] \,\big|\, \deg f = k-l, \quad f^{\sharp}|_{\mathrm{sh}_j} = f|_{\mathrm{sh}_j} = 0 \quad \forall j\}\,.$$

is isomorphic to $Ari^{pol}_{\underline{al},\underline{al}}$ over $\mathbb{Q}$.

Ekma and Carma sub Lie algebras

The so called Ekma moulds

$$\xi_r(u_1) = u_1^{r-1}, \qquad r \geqslant 3 \text{ and odd}$$

generate a Lie Algebra $\mathfrak{E} \subset Ari^{pol}_{\underline{al},\underline{al}}$. The multiplication $ari : \mathfrak{E}^1 \times \mathfrak{E}^1 \to \mathfrak{E}^2$ factors through $\mathfrak{E}^1 \wedge \mathfrak{E}^1$, which is spannend by $\xi_r(u_1)\xi_s(u_2) - \xi_r(u_2)\xi_s(u_1)$, thus

$$\mathfrak{E}^1 \wedge \mathfrak{E}^1 = \{p \in \mathbb{Q}[u_1, u_2] \,|\, p(u_1, u_2) + p(u_2, u_1) = 0, \quad p(\pm u_1, \pm u_2) = p(u_2, u_1)\}.$$

The map $ari : \mathfrak{E}^1 \wedge \mathfrak{E}^1 \to \mathfrak{E}^2$ induced by $ari(\xi_r \wedge \xi_s) = ari(\xi_r, \xi_s)$ equals

$$ari(p(u_1, u_2)) = p(u_1, u_2) + p(u_1 + u_2, u_1) + p(u_2, u_1 + u_2).$$

Now one observes

$$\ker(ari) = W^+ = \{ \text{ even period polynomials for } \mathrm{SL}_2(\mathbb{Z})\}$$

There is another Lie algebra $\mathfrak{C} \subset Ari^{pol}_{\underline{al},\underline{al}}$ generated by the Carma moulds $\kappa_f(u_1, u_2, u_3, u_4)$, where the dependence on $f \in W^+$ is quite complicated.

Conjecture (Ecalle)

(i) The relations in $\mathfrak{E}$ are generated in depth 2 by even period polynomials as above.

(ii) The Lie algebra $\mathfrak{C}$ is free.

(iii) $Ari^{pol}_{\underline{al},\underline{al}}$ is generated by $\mathfrak{E}$ and $\mathfrak{C}$, and there are no relations between them.

Consequences

If we assume in addition that there is no higher homology, then the abelianisation of the universal enveloping algebras would have the following Hilbert-Poincare series:

$$\sum_{k,l} \dim \mathrm{gr}^{\mathrm{W,D}}_{k,l} \mathfrak{A}_{\mathfrak{E}} x^k y^l = \frac{1}{1 - O(x)y + S(x)y^2}$$

$$\sum_{k,l} \dim \mathrm{gr}^{\mathrm{W,D}}_{k,l} \mathfrak{A}_{\mathfrak{C}} x^k y^l = \frac{1}{1 - S(x)y^4}$$

$$\sum_{k,l} \dim \mathrm{gr}^{\mathrm{W,D}}_{k,l} \mathfrak{A}_{Ari^{pol}_{\underline{al},\underline{al}}} x^k y^l = \frac{1}{1 - O(x)y + S(x)y^2 - S(x)y^4}$$

Computational evidence was provided by S. Carr.

alternal, swap-invariant, neg-invariant bimoulds

Observe the natural map

$$\iota : Ari^{pol}_{\underline{al},\underline{al}} \to Bari^{pol}_{\underline{al},swap}$$

given by $\iota(A)(w) = A(u) + swap(A)(v)$. In particular

$$\xi_s \binom{u_1}{v_1} = \iota(\xi_s) = \xi_s(u_1) + \xi_s(v_1).$$

Proposition

The map $\delta : Bari^{pol}_{\underline{al},swap} \to Bari^{pol}_{\underline{al},swap}$ given in depth l by multiplication with $u_1 v_1 + ... + u_l v_l$ satisfies the Leibniz rule, i.e.

$$\delta ari(A, B) = ari(\delta A, B) + ari(A, \delta B).$$