Report

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Identities arising from coproducts on MZVs and MPLs

1 Introduction

Multiple zeta values (MZVs) are a highly mysterious set of real numbers defined by the following nested sums

$$\zeta(s_i,\dots,s_k) \coloneqq \sum_{1\leq n_1<\cdots<n_k} \frac{1}{n_1^{s_1}\cdots n_k^{s_k}}\,,$$

for $s_i > 0 \in \mathbb{Z}$, which one can view as a multi-variable generalisation of the Riemann zeta values. For convergence we require $s_k \geq 2$.

The main source of interest in studying MZVs occurs in trying to gain a full understanding their sructure and of the relations they satisfy. There are many folklore conjectures [2] describing the structure of MZVs, which so far remain unproven, such as the *direct sum* conjecture which claims the $\mathbb{Q}$-vector space of MZVs is weight graded, the *dimension conjecture* giving $\dim_{\mathbb{Q}} Z_k = d_k$, where d_k satisfies the recurrence relation $d_k = d_{k-2}+d_{k-3}$, $d_2 = d_3 = d_4 = 1$, and the *basis conjecture* [12] which refines the dimension conjecture with a proposed basis $\{\zeta(w) \mid w \text{ contains only 2s and 3s}\}$.

Recently some progress on these conjectures has been made from the *motivic* [4, 5, 10]viewpoint, wherein one obtains a purely algebraic lifting of the MZVs to motivic MZVs capturing the essential properties of but eschewing the analytic awkwardness. By definition one gets the weight grading, since motivic MZVs live in a Hopf algebra graded by weight. Brown and Zagier have established that basis conjecture for motivic MZVs, and so deduce from the period map that the proposed basis is certainly a spanning set for weight k MZVs [4, 14]. This gives another proof of the known inequality $\dim_{\mathbb{Q}} Z_k \leq d_k$. Since it is not even know that $\dim_{\mathbb{Q}} Z_5 > 1$, these conjecture are still far from being resolved for real MZVs.

Living in a Hopf algebra entails the existence of a coproduct on motivic MZVs, a structure which conjecturally exists on the real MZVs, but is not readily apparent. This coproduct provides a much more rigid structure on the set of motivic MZVs, allowing new techniques of proof.

Multiple zeta values can be viewed as special values of multiple polylogarithms (MPLs), a set of functions defined as follows

$$\mathrm{Li}_{s_1,\dots,s_k}(z_1,\dots,z_k) \coloneqq \sum_{1\leq n_1<\cdots<n_k} \frac{z_1^{n_1}\cdots z_k^{n_k}}{n_1^{s_1}\cdots n_k^{s_k}}\,,$$

so that $\zeta(s_1,\dots,s_k) = \mathrm{Li}_{s_1,\dots,s_k}(1,\dots,1)$. These functions are a multi-variable generalisation of *polylogarithms*, themselves a generalisation of the ordinary logarithm function.

Typically one is interested in finding functional equations for polylogarithms and multiple polylogarithms, in no small part due to their connection to algebraic K-theory via Zagier's conjecture – sufficiently general functional equations for the polylogarithms should lead to an explicit description of K groups in terms of generators and relations. Goncharov's work on the trilogarithm, and its generic functional equation arising from the triple ratio, has resolved the $n = 3$ case, giving a description of $K_5(F)$, and expressing $\zeta_F(3)$ n terms of Li_3 [11].

At weight 4 or higher, polylogarithms alone are no longer sufficient to express all arising iterated integrals; one genuinely needs to incorporate multiple polylogarithm into the setup, and understand their identities and functional equations alongside the polylogarithms. Moreover, these kind of special functions arise in numerous calculations in High Energy Physics, usually producing exceedingly complicated answers. A good understanding of the relations and functional equations between different MPLs is essential to drastically simplifying such calculations, hence the interest.

To a multiple polylogarithm, one can attach an algebraic invariant called the *symbol* which captures the differential properties of the function. The symbol can be built up iteratively from the total derivative of the function, but also has descriptions in terms of trees, in terms of polygons, and in terms of maximally iterating a coproduct. [13, 10, 8]

The symbol reflects in an algebraic manner the functional equations MPLs satisfy. The symbol of a functional equation should always simplify to 0 using the rules of tensor calculus. This can be reverse engineered to derive functional equations by taking a linear combination of suitably many arguments, and solving to make the resulting symbol identically 0.

2 Cyclic insertion conjecture on MZVs

The cyclic insertion conjecture of Borwein, Bradley, Broadhurst, and Lisoněk [1] claims the following identity holds on MZVs

Conjecture 2.1 (Cyclic insertion)**.**

$$\sum_{\textit{cyclic shifts of } a_i} \zeta(2^{a_0}, 1, 2^{a_1}, 3, \ldots, 1, 2^{a_{2n-1}}, 3, 2^{a_{2n}}) \stackrel{?}{=} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$$

So far, the only explicit identity which have been proven in this direction is the Bowman-Bradley theorem [3], stating

Theorem 2.2 (Bowman-Bradley)**.**

$$\begin{aligned}\sum_{\textit{compositions } a_0 + \cdots + a_{2n} = N} \zeta(2^{a_0}, 1, 2^{a_1}, 3, \ldots, 1, 2^{a_{2n-1}}, 3, 2^{a_{2n}}) &= \zeta(2^N \sqcup \{1,3\}^m) \\ &= \frac{1}{2m+1}\binom{N+2m}{N}\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\end{aligned}$$

By making use of the motivic MZV framework, I have shown that inserting only permutations of fixed blocks 2^{a_i} is sufficient to get a rational multiple of π^{wt}, so that the Bowman-Bradley theorem breaks up into smaller subsums.

Theorem 2.3 (C, Symmetric Insertion, [6])**.**

$$\sum_{\textit{permutations of } a_i} \zeta(2^{a_0}, 1, 2^{a_1}, 3, \ldots, 1, 2^{a_{2n-1}}, 3, 2^{a_{2n}}) \in \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\mathbb{Q}$$

A similar-looking conjectural family of identities is presented by Hoffman [2, Equation 5.6]

Conjecture 2.4 (Hoffman)**.**

$$2\zeta(3,3,2^n) - \zeta(3,2^n,1,2) = -\zeta(2^{3+n}) \stackrel{?}{=} -\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$$

I can also give a motivic proof of this identity, although like Symmetric Insertion, it is only up to a rational constant. This naturally leads to a much larger family of identities resembling symmetric insertion above

Theorem 2.5.

$$\sum_{j=0}^{2n} \sum_{\textit{permutations of } a_i} (-1)^j \zeta(2^{a_0}, 3, \ldots, 2^{a_{2n-j}}, 3, 2^c, \{1,2\}, 2^{a_{2n-j+1}}, \ldots, \{1,2\}, 2^{a_{2n}}) \in \pi^{\mathrm{wt}}\mathbb{Q}$$

Numerical evaluation, and searching for identities using integer relation algorithms suggests that this is just a symmetrised version of a more precise identity, as cyclic insertion is to symmetric insertion.

Conjecture 2.6.

$$\sum_{j=0}^{2n}(-1)^j\zeta(2^{a_j},3,\ldots,2^{a_{2n-1}},3,2^{a_{2n}},\{1,2\},2^{a_0},\ldots,\{1,2\},2^{a_{j-1}}) \overset{?}{=} (-1)^n\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$$

These examples, along with some others found from the coproduct on motivic MZVs, such as

$$2\zeta(1,3,3,3)+2\zeta(3,3,1,3)-\zeta(3,1,3,1,2)\in\pi^{10}\mathbb{Q}\,,$$

serve as a jumping off point form which to investigate and formulate a generalised cyclic insertion conjecture.

Conjecture 2.7 (Generalised cyclic insertion)**.** *Let B be the set of MZVs whose arguments, and their duals, consist entirely of 1s, 2s and 3s. Define the operator X on these MZVs as follows:*

$$\begin{aligned}
&\zeta(2^a,1,2^b,3,w)\mapsto\zeta(w,1,2^a,3,2^b)\\
&\zeta(2^a,3,w)\mapsto-\zeta(w,1,2,2^a)\\
&\zeta(2^{a_0},1,2,2^{a_1},\ldots,1,2,2^{a_k},1,2^{a_{k+1}},3,w)\mapsto(-1)^k\zeta(w,1,2^{a_0},3,2^{a_1},3,\ldots,3,2^{a_{k+1}})\,.
\end{aligned}$$

Let $z\in B$ be such an MZV, and apply the operator X continually to find the orbit $\mathcal{O}_X(z)$. Then

$$\sum\mathcal{O}_X(z)\overset{?}{=}\mathrm{sgn}((-1)^{(\#3(z)-\#3(\mathrm{dual}(z)))/2})\frac{|\mathcal{O}_X(z)|}{\#3(\mathrm{dual}(z))+\#3(z)+1}\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,,$$

where one should view $\mathrm{sgn}(\pm\mathrm{i}):=0$*. (Here* dual *refers to MZV corresponding to z by* dualiy *[2, Theorem 4.1].)*

An explicit proof of this unfortunately remains elusive, particularly since it generalises two already conjectural results. Thus I am currently investigating motivic proofs of various symmetrisations of the generated identities, something I have already had success with in previous cases above.

I can show generally that some sufficiently symmetrised (though not trivially so) version of the identity indeed holds at even weight. Some particular examples, other than those above, are as follows:

$$\begin{aligned}
&\zeta(2^n,1,3,3,1,2)+\zeta(3,1,2,1,2^n,3)-\zeta(1,2,1,2^n,3,1,2)+\\
&\quad+\zeta(1,2,1,3,3,2^n)-\zeta(3,2^n,1,3,3)\in\frac{\pi^{2n+10}}{(2n+11)!}\mathbb{Q}\,,
\end{aligned}$$

which gives one of the cyclic insertion identities on the nose, in this case. And

$$\sum_{\text{compositions } a_i\,=\,M}\zeta_X(\{1,3\}^N,3,3\mid a_0,\ldots,a_{2N+2})\in\pi^{\mathrm{wt}}\mathbb{Q}\,,$$

which can be seen as an analogue for the Bowman-Bradley result which holds for $\zeta(\{1,3\}^m)$.

(Here I use the notation $\zeta_X(w\mid\{a_i\})$ to mean the cyclic insertion identity generated by inserting a_i in the i-th gap of the argument string w.)

3 Identities and relations between weight ≥ 5 MPLs

The weight 4 case has been studied in detail by Gangl, who is assembling a compendium of functional equations and symmetries satisfies by the various weight 4 MPLs [9](or more precisely their corresponding iterated integrals, for simplicity). I am in undertaking a similar analysis of the weight 5 case, with forays into higher weight cases if possible.

Initially a good choice of arguments to analyse consists of cross ratios. Products of cross ratios can enter in the more complicated cases. After computing the symbol, one work at various levels of refinement to produce successively more precise identities. Firstly work modulo δ which kills products and Li_n terms giving the top 'slice' of an identity. One identity that I find initially is

$$I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{x}, \tfrac{1}{y}) \equiv_\delta 0\,.$$

Make this more precise by finding the Li_5 terms. To do this, compute the symbol modulo $\sqcup\!\sqcup$, which kills only products, and allows Li_n terms to survive. I find

$$I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{x}, \tfrac{1}{y}) \equiv_{\sqcup\!\sqcup} -\mathrm{Li}_5(x) - 4\,\mathrm{Li}_5(\tfrac{x}{y}) + \mathrm{Li}_5(y)\,.$$

Lastly on the symbol level, one can search for the missing product terms to build up the exact identity. For example:

$$\begin{aligned}
&I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{x}, \tfrac{1}{y}) \\
&+ (\mathrm{Li}_5(x) + 4\,\mathrm{Li}_5(\tfrac{x}{y}) - \log(\tfrac{x}{y})\,\mathrm{Li}_4(\tfrac{x}{y})) \\
&+ \sum_{i=0}^{4} \tfrac{1}{i!}(-\log(x))^i\,\mathrm{Li}_{5-i}(y) - \frac{1}{5!}(\log^5(\tfrac{x}{y}) - \log^5(x)) \quad \equiv_{\mathcal{S}} \quad 0
\end{aligned}$$

By itself this is not enough to give a completely correct numerically testable identity since the symbol does not detect contributions of the form constant $\times$ lower weight. These terms can be investigated using the coproduct Δ on MPLs, to build up a successive slices of the numerically testable identity:

$$\begin{aligned}
&I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{x}, \tfrac{1}{y}) \\
&\quad + (\mathrm{Li}_5(x) + 4\,\mathrm{Li}_5(\tfrac{x}{y}) - \log(\tfrac{x}{y})\,\mathrm{Li}_4(\tfrac{x}{y})) \\
&\quad \tfrac{1}{5!}(-\log^5(\tfrac{x}{y}) + \log^5(x)) + \widetilde{\mathrm{Li}}_5(x,y) \\
&\\
&\quad + i\pi(-\tfrac{1}{4!}\log^4(x) + \widetilde{\mathrm{Li}}_4(x,y)) \\
&\quad + \tfrac{-2\pi^2}{6}(\tfrac{1}{3!}(\log^3(\tfrac{x}{y}) + \log^3(x)) + \widetilde{\mathrm{Li}}_3(x,y)) \\
&\quad + \tfrac{-2\pi^4}{90}(\tfrac{1}{1!}(3\log(\tfrac{x}{y}) + \log(x)) + \widetilde{\mathrm{Li}}_1(x,y)) = 0\,.
\end{aligned}$$

Theorem 3.1. *A similar symbol level identity holds for all iterated integrals $I_{a,b}(x,y)$, including a precise description of the product terms and Li_n terms. A similar candidate numerically testable identity can be given for $I_{n,1}(x,y)$.*

The above identity is just one example arising from cross ratio arguments. I am in the process of assembling a compendium of similar identities for all of the weight 5+ iterated integrals ranging from the depth 2 integrals $I_{4,1}, I_{3,2}, I_{2,3}$ and $I_{1,4}$ through to the most generic integral the quintuple-logarithm $I_{1,1,1,1,1}$.

Part of this also includes investigating relations between *different* iterated integrals. For example, I have found expression for all weight 5 depth 3 integrals purely in terms of $I_{3,2}$ and $I_{3,1,1}$. Combining this with Dan's reduction method [7] gives an expression for any weight 5 MPL purely in terms of $I_5, I_{3,2}$ and $I_{3,1,1}$, showing these three functions suffice.

Theorem 3.2. *Any weight 5 MPL can be expressed in terms of $I_5, I_{3,2}$ and $I_{3,1,1}$ (and products of lower weight).*

It is expected that the index 1 can always be eliminated from an MPL, so one should be able to find an expression in terms of I_5 and $I_{3,2}$ only. This result reduces the question to tackling one specific case at weight 5: finding $I_{3,1,1}$ in terms of $I_{3,2}$, which is potentially a more tractable problem.

As another line of exploration, Goncharov gives a schematic plan of how to derive a functional equation for Li_5 from expressions for particular elements in terms of Li_5. [11] Goncharov gave a similar schematic plan for Li_4, and the resulting functional equation has been found by Gangl, after expressing Goncharov's element in terms of Li_4 of products of up to 8 cross ratios. I intend to make a similar attempt on the Li_5 case .

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