Polylogarithms and Multiple Zeta Values

Michel Petitot
University of Lille I

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[summary by Bruno Salvy]

The *polylogarithm* is defined by the series

$$L_{x_0^{n_1-1}x_1\cdots x_0^{n_k-1}x_1}(z) := \sum_{n_1>\cdots>n_k>0} \frac{z^{n_1}}{n_1^{s_1}\cdots n_k^{s_k}}.$$

The convergence of this series at 1 is granted when $s_1 > 1$, and the limit is denoted $\zeta(s_1,\ldots,s_k)$ and is called a *multiple zeta value* since it extends the classical Riemann zeta function. The number $\sum s_i$ is called the *weight* of the polylogarithm or multiple zeta.

Many polynomial identities relating multiple zeta values at integers are known. For instance, reorganizing double sums yields the following identity between multiple zetas of weight 4:

$$(1) \qquad \zeta(2,2) = \sum_{n_1>n_2>0} \frac{1}{n_1^2 n_2^2} = \frac{1}{2}\left(\sum_n \frac{1}{n^2}\right)^2 - \frac{1}{2}\sum_n \frac{1}{n^4} = \frac{1}{2}(\zeta(2)^2 - \zeta(4)).$$

This could be simplified further using the well-known values of ζ at even integers.

This is a very active and diverse area. The reader is encouraged to consult [1, 2] for surveys of many beautiful results, generalizations and conjectures. One of the most famous conjectures is the following.

Conjecture 1 (Zagier). *The set of multiple zeta values $\zeta(s_1,\ldots,s_k)$ with s_i positive integers, $s_1 \geq 2$ and $s_1+\cdots+s_k \leq n$ generates a vector space over $\mathbb{Q}$ whose dimension d_n obeys*

$$d_{n+3} = d_{n+1} + d_n, \qquad d_1 = 0, \quad d_2 = d_3 = 1.$$

Note that since even the irrationality of $\zeta(5)$ is still unproven, this conjecture is completely out of reach. Even a proof that this sequence gives an upper bound is still to be found.

1. Shuffle and Stuffle

The manipulation leading to identity (1) is a special case of a more general mechanism involving products of multiple sums. By considering how indices in multiple sums can be reorganized, it is natural to define the *stuffle product* of two words over $\mathbb{N}$. (Stuffle is a contraction of "shuffle" and "stuff".) Using lowercase symbols to denote letters and capital symbols to denote words, this is the formal sum defined recursively by

$$\epsilon \star W = W \star \epsilon = W, \qquad aS \star bT = a(S\star bT) + b(aS\star T) + (a+b)(S\star T).$$

This definition is motivated by the following important *stuffle relation*:

$$\zeta(A)\zeta(B) = \sum_{S\in A\star B} \zeta(S).$$

A simple example is $\zeta(2)\zeta(3) = \zeta(2,3) + \zeta(3,2) + \zeta(5)$. Another one is the identity (1) which is obtained from $(2) \star (2) = 2(2,2) + 2(4)$.

In the same way as the stuffle product arises in the reorganization of multiple sums, multiple integrals lead to considering the *shuffle product* of words over the alphabet $X = \{x_0, x_1\}$. This is defined by the same formula as the stuffle product except that the last term in the sum is omitted. A bijection between words over $\mathbb{N}^\star$ and words of $X^\star x_1$ is provided by the encoding

$$(s_1, \dots, s_k) \leftrightarrow x_0^{s_1-1} x_1 \cdots x_0^{s_k-1} x_1.$$

This makes it possible to extend the shuffle product to these words. For instance,

$$(2) ш (2) \mapsto x_0x_1 ш x_0x_1 = 2x_0x_1x_0x_1 + 4x_0x_0x_1x_1 \mapsto 2(2,2) + 4(3,1),$$

$$(2) ш (3) \mapsto x_0x_1 ш x_0x_0x_1 = 6x_0^3x_1^2 + 3x_0^2x_1x_0x_1 + x_0x_1x_0^2x_1 \mapsto 6(4,1) + 3(3,2) + (2,3).$$

The following integral representation is then proved by induction

$$(2) \qquad L_{x_1}(z) = \log \frac{1}{1-z} = \int_0^z \frac{dt}{1-t}, \qquad L_w(z) = \begin{cases} \int_0^z \frac{dt}{t} L'_w(t), & \text{if } w = x_0w', \\ \int_0^z \frac{dt}{1-t} L'_w(t), & \text{if } w = x_1w'. \end{cases}$$

The recursive definition of the shuffle now reads $UV = \int U'V + \int UV'$, whence the *shuffle relation*:

$$L_A(z)L_B(z) = \sum_{S \in A ш B} L_S(z).$$

Setting $z = 1$ in these identities yields new identities concerning multiple ζ values. Our examples above thus lead to $\zeta(2)^2 = 2\zeta(2,2) + 4\zeta(3,1)$, $\zeta(2)\zeta(3) = 6\zeta(4,1) + 3\zeta(3,2) + \zeta(2,3)$.

Conjecture 2. *All known relations concerning multiple zeta values follow from the stuffle product of multiple zetas and the shuffle product of polylogarithms specialized at 1.*

This has been checked up to weight 12 [3], and the set of identities thus obtained coincides with the bound provided by Zagier's conjecture.

2. Monodromy and Consequences

A first step towards proving the conjecture above is provided by the following theorem.

Theorem 1 ([4]). *The ideal of algebraic relations between polylogarithms at z is generated by the shuffle relations.*

A *Lyndon word* is a non-empty word which precedes its strict right factors in the lexicographic order. A classical theorem due to Radford states that the Lyndon words form a basis of the shuffle algebra. This leads to the following result.

Corollary 1. *The polylogarithms indexed by Lyndon words form a transcendence basis of the polylogarithms. In particular, the classical polylogarithms $\mathrm{Li}_k = L_{x_0^k x_1}$ are algebraically independent.*

This theorem is proved for relations involving polylogarithms of weight bounded by a fixed number. Using the shuffle relations, any polynomial in polylogarithms can be reduced to a linear combination of polylogarithms. Since the shuffle relations form a Gröbner basis for the total degree order (degrevlex), any polynomial which is not in the ideal is thus reduced to a *nonzero* linear combination. The theorem is thus reduced to proving that the polylogarithms are *linearly* independent. This is done by computing the monodromy of polylogarithms as we now describe.

It turns out to be convenient to prove a more general theorem where polylogarithms with indices ending in x_0 are allowed. Consistency with the shuffle relations is achieved with

$$L_{x_0}(z) := \int_1^z \frac{dt}{t} = \log z, \qquad L_{x_0^m}(z) := \int_1^z \frac{dt}{t} L_{x_0^{m-1}}(t) = \frac{1}{m!}\log^m z.$$

At $z=0$, the situation is simple: a word ending with x_1 corresponds to an analytic polylogarithm, whence a trivial monodromy. An easy induction on the weight shows that all words ending in x_0 can be rewritten as a sum of shuffles of powers of x_0 and words ending in x_1. Here are the corresponding relations up to weight 3:

$$L_{x_1x_0} = L_{x_1}L_{x_0} - L_{x_0x_1}, \quad L_{x_1^2x_0} = L_{x_1^2}L_{x_0} - L_{x_1x_0x_1} - L_{x_0x_1^2},$$
$$L_{x_0x_1x_0} = L_{x_0x_1}L_{x_0} - 2L_{x_0^2x_1}, \quad L_{x_1x_0^2} = L_{x_1}L_{x_0^2} - L_{x_0x_1}L_{x_0} + L_{x_0^2x_1}.$$

Let $\mathcal{M}_0 f(z)$ be $f(ze^{2i\pi})$; applying $\mathcal{M}_0 - \mathrm{Id}$ on the right-hand sides of these identities only affects the $L_{x_0^k}$. Their monodromy follows from $(\mathcal{M}_0 - \mathrm{Id})L_{x_0} = 2i\pi$. Another shuffle thus shows that

$$(\mathcal{M}_0 - \mathrm{Id})L_{Ux_0} = 2i\pi L_U + \sum_V \mu_V L_V, \qquad (\mathcal{M}_0 - \mathrm{Id})L_{Ux_1} = 0,$$

where the words V in the sum all have weight smaller than the weight of U.

We now proceed to prove the analogous property at 1 with $\mathcal{M}_1 f(1-z) := f((1-z)e^{2i\pi})$:

$$(\mathcal{M}_1 - \mathrm{Id})L_{Ux_1} = -2i\pi L_U + \sum_V \mu_V L_V, \qquad (\mathcal{M}_1 - \mathrm{Id})L_{Ux_0} = 0. \tag{3}$$

At $z=1$, words ending with x_0 correspond to polylogarithms that are analytic there, hence, have a trivial monodromy. This is the second identity. The situation is slightly more complicated than at the origin because of divergence. As above, an induction on the weight shows that all words beginning with x_1 can be rewritten as a sum of shuffles of powers of x_1 and words beginning with x_0. The monodromy of $L_{x_1^k}$ follows from that of the logarithm. The remaining words are those beginning with x_0 and ending with x_1. Consider the path consisting of a straight line from z to a circle of radius ϵ around 1, turning around 1 in the anti-clockwise direction and coming back to z. Then Cauchy's theorem implies that

$$(\mathcal{M}_1 - \mathrm{Id})L_{x_0Ux_1}(z) = \lim_{\epsilon\to 0}\int_{1-\epsilon}^z \frac{dt}{t}(\mathcal{M}_1 - \mathrm{Id})L_{Ux_1}(t) + \lim_{\epsilon\to 0}\oint_{|1-t|=\epsilon}\frac{dt}{t}L_{Ux_1}(t).$$

Another induction shows that the rightmost integral tends to 0, while convergence of L_{Ux_1} at 1 reduces the first limit to

$$\int_1^z \frac{dt}{t}(\mathcal{M}_1 - \mathrm{Id})L_{Ux_1}(t).$$

This makes it possible to compute all the monodromies of words ending in x_1 and proves (3). Here are the corresponding relations up to weight 3, using p to denote $2i\pi$:

$$(\mathcal{M}_1 - \mathrm{Id})L_{x_1^k} = \sum_{j=1}^k L_{x_1^{k-j}}\frac{(-p)^j}{j!}, \qquad (\mathcal{M}_1 - \mathrm{Id})L_{x_0x_1} = -pL_{x_0}, \quad (\mathcal{M}_1 - \mathrm{Id})L_{x_0^2x_1} = -pL_{x_0^2},$$

$$(\mathcal{M}_1 - \mathrm{Id})L_{x_0x_1^2} = -p(L_{x_0x_1} - \zeta_{x_0x_1}) + \frac{p^2}{2}L_{x_0}, \quad (\mathcal{M}_1 - \mathrm{Id})L_{x_1x_0x_1} = 2L_{x_0x_1^2} - pL_{x_1x_0} - 2p\zeta_{x_0x_1}.$$

The proof of Theorem 1 is concluded by considering the maximal weight involved in a minimal non-trivial linear combination: applying both operators $(\mathcal{M}_0 - \mathrm{Id})$ and $(\mathcal{M}_1 - \mathrm{Id})$ leads to linear relations of smaller weight, that have to be trivial.

3. Changes of Variables

The group of six rational functions z, $1-z$, $1/z$, $1/(1-z)$, $1-1/z$, $z/(1-z)$ permutes the singularities 0, 1, ∞. If h is an element of this group, then

$$L_{xU}(h(z)) = \int_0^{h(z)} L_U(t)w_x(t)\,dt = \int_{h^{-1}(0)}^{z} L_U(h(s))w_x(h(s))h'(s)\,ds.$$

It turns out that for all h in the group and all $x \in \{x_0, x_1\}$, $w_x(h(s))h'(s)$ can be rewritten as a linear combination of ds/s and $ds/(1-s)$. Thus by induction, all polylogarithms at $h(z)$ can be rewritten in terms of polylogarithms at z. For the classical dilogarithm $\mathrm{Li}_2 = L_{x_1x_0}$, we get

$$\mathrm{Li}_2(1-z) + \mathrm{Li}_2(z) = L_{x_0}(z)L_{x_1}(z) + \zeta(2),\ \mathrm{Li}_2(z) - \mathrm{Li}_2(1-z^{-1}) = L_{x_0}(z)L_{x_1}(z) + \zeta(2) + L_{x_0^2}(z).$$

Setting z to $1/2, \pm\phi, \pm 1/\phi, 1+\phi, 1-1/\phi$, where ϕ is the golden ratio, yields the only known values of Li_2 in closed form.

4. Noncommutative Generating Function

All the inductions mentioned here are conveniently handled by introducing the noncommutative generating function $L(z) = \sum L_W(z)W$ where the sum is over all words of $\mathcal{X} = \{x_0, x_1\}^\star$. The integral representation of polylogarithms is equivalent to a linear differential equation:

$$\frac{d}{dz}L(z) = \left(\frac{x_0}{z} + \frac{x_1}{1-z}\right)L(z).$$

A consequence of the rewriting of words ending by x_0 is that all polylogarithms except $L_{x_0}^k$ tend to 0 at the origin. This leads to the initial condition $L(\epsilon) = e^{\ln \epsilon x_0} + O(\epsilon^{1-\delta})$, for $\epsilon \to 0$, where δ is an arbitrarily small real number. The shuffle relation then implies that this generating function is a *Lie exponential*. A noteworthy consequence is that it can be factored as a product of Lie exponentials indexed by Lyndon words, which turns out to yield an efficient algorithm for computing identities [3].

The inductions used in the monodromy computations translate very explicitly into

$$\mathcal{M}_0 L(z) = L(z)e^{2i\pi x_0}, \qquad \mathcal{M}_1 L(z) = L(z)Z^{-1}e^{-2i\pi x_1}Z,$$

where Z is very close to being the generating function of the multiple zeta values: it is the unique Lie exponential such that

$$(Z|x_0) = (Z|x_1) = 0, \qquad (Z|x_0Wx_1) = \zeta_{x_0Wx_1}, \quad W \in \mathcal{X}.$$

Similarly, the changes of variables can be interpreted at the level of $L(z)$ [5].

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