Special functions, their numerical representations and transcendentals in QCD

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Polylogarithms

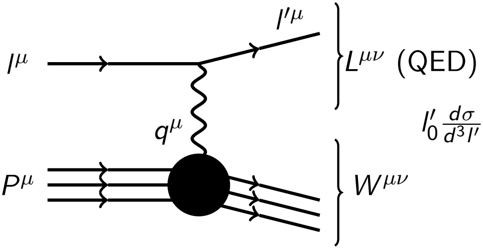
This talk is an overview of the ongoing problem of special functions in perturbative QCD and their numerical properties.

1. Background to work
2. Review the basic definitions and properties
3. ‘Goncharov’s conjecture’ (excluding the symbol)
4. Numerical evaluation
5. PSLQ and transcendentals

(My talks were based around computer algebra approaches to problems.)

Heavy Flavour Wilson Coefficients

Our work concerns summation problems found from 3-loop parton distribution functions (PDFs). Recall the DIS experiment,



$$l'_0 \frac{d\sigma}{d^3 l'} = \frac{1}{4 l \cdot P} \frac{\alpha^2}{q^2} L_{\mu\nu} W^{\mu\nu}$$

DIS diagram Factorisation Cross-section

$$W^{\mu\nu} = \frac{1}{2x}\left(g^{\mu\nu} - \frac{q^{\mu}q^{\nu}}{q^2}\right) F_L(x, Q^2) + \frac{2x}{Q^2}\left(P^{\mu}P^{\nu} + \frac{q^{\mu}P^{\nu} + q^{\nu}P^{\mu}}{2x} - \frac{Q^2}{4m^2} g^{\mu\nu}\right) F_2(x, Q^2)$$

Heavy Flavour Wilson Coefficients

The structure functions are written in terms of the (unknown) PDF, f_j, and a perturbative piece; the Wilson coefficients $\mathbb{C}_{i,j}$,

$$F_i(x) = \sum_j \int \frac{dz}{z} \mathbb{C}_{i,j} \left(\frac{x}{z}\right) f_j(z),$$

$i \in \{2, L\}$ and j runs over all (anti-)quarks and the gluon. There is a well established literature where light flavour contributions are known to 3-loops, heavy contributions to 2-loops.

1-loop Many contributors; Witten '76, Babcock & Sivers '78, Shifman, Vainshtein & Zakharov '78, Leveille & Weiler '79, Glück & Reya '79, Glück, Hoffmann & Reya '82.

2-loop First by Laenen, van Neerven, Riemersma & Smith '93
Using integration by parts and $Q^2 \gg m^2$; Buza, Matiounine, Smith, Migneron & van Neerven '96. Using ${}_pF_q$'s and to order $\alpha_s \epsilon$ Bierenbaum, Blümlein, Klein & Schneider '08, Bierenbaum, Blümlein & Klein '09

3-loop For $Q^2 \gg m^2$ fixed moments $N = 2..10+$
$A_{qq,Q}^{NS}$, $A_{qq,Q}^{TR}$, $A_{qq,Q}^{PS}$ Ablinger et al. '14
$A_{qg,Q}$ manuscript in preparation Ablinger et al. '14
$A_{gg,Q}$ proportional to $n_f T_F^2 C_{A/F}$ Ablinger et al. '14
$+ \ldots$

Here $A_{i,j}$ appears which is the heavy flavour contribution.

Heavy Flavour Wilson Coefficients

The Wilson coefficients may be written out as a sum of light and heavy contributions,

$$\mathbb{C}_{j,(2,L)}\left(N, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}\right) = C_{j,(2,L)}\left(N, \frac{Q^2}{\mu^2}\right) + H_{j,(2,L)}\left(N, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}\right)$$

and if $Q^2 \gg m^2$ one my factorise the heavy part in terms of the light part Buza, Matiounine, Smith, van Neerven

$$H_{j,(2,L)}\left(N, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}\right) = \sum_i C_{i,(2,L)}\left(N, \frac{Q^2}{\mu^2}\right) A_{ij}\left(\frac{m^2}{\mu^2}, N\right)$$

We have been computing the heavy flavour 3-loop contributions at large $\xi = \frac{Q^2}{m_c^2}$.

Heavy Flavour Wilson Coefficients

Recall that the PDF is introduced as a Mellin convolution,

$$F_i(x) = \sum_j \int \frac{dz}{z} \mathbb{C}_{i,j}\left(\frac{x}{z}\right) f_j(z) = \sum_j \mathbb{C}_{i,j} * f_j.$$

Thus by taking the Mellin transform,

$$\mathcal{M}[g](N) = \int_0^1 dx x^{N-1} g(x) \quad N \in \mathbb{Z}^+$$

things simplify greatly. In Mellin space Feynman diagrams contributing to the Wilson coefficients $C_{i,j}$ become rational in the Mellin parameter N and definite sums involving N. For experiment, the inverse transform of results must be computed. (Less relevant today but key to our wider project.)

Polylogarithms

All of this is to motivate the main topic of the talk; polylogarithms.

- Having computed the Wilson coefficients one needs an efficient evaluation to perform fits and extract PDFs.
- The problem is general; higher-loop calculations lead to polylogarithms that need to be evaluated.
- Therefore one should study the functions in their own right to understand cross-sections better and to be able to evaluate them.

Polylogarithms

Parameter integrals

To compute the Wilson coefficients one must compute Feynman diagrams (with the additional feature of an operator insertion). The standard practice is to introduce Feynman parameters,

$$\frac{1}{A_1 \cdots A_m} = \Gamma(m) \int_0^1 dx_1 \cdots dx_m \frac{\delta(x_1 + \cdots + x_m - 1)}{(x_1 A_1 + \cdots x_m A_m)^m}$$

One may apply the δ-function which introduces a step function Θ,

$$x_1 = 1 - x_2 - \cdots - x_m \in (0, 1),$$
$$\int_0^1 dx_2 \cdots dx_m \frac{\Theta(1 - x_2 - \cdots - x_m)}{([1 - x_2 - \cdots - x_m] A_1 + \cdots x_m A_m)^m}$$

Polylogarithms

Letters

This can be re-arranged via some changes of variables into a sum of nested integrals,

$$\int_0^1 dt_1 f(t_1) \int_0^{t_1} f(t_2) dt_2 \cdots \int_0^{t_n - 1} dt_n f(t_n).$$

What is not clear is how to choose the f_i. Essentially the most basic objects of interest are,

$$\frac{1}{x - a_i}.$$

The a_i are referred to as letters and intuitively represent dimensionless combinations of scales arising in the problem. Iterated integrals over letters f_i are known as polylogarithms with various prefixes.

Polylogarithms

Example

This certainly does not cover all possible Feynman diagrams — there are parameter integrals that can not be cast in terms of nested integrals over f_i. However one can obtain a lot of diagrams this way and these objects are already very general. While elementary this is sufficiently important to warrant an example. Consider,

$$\begin{aligned}
\frac{1}{ABC} &= \int_0^1 dx_i \frac{\delta(1-x_1-x_2-x_3)}{[x_1A+x_2B+x_3C]^3}, \\
&= \int_0^1 dx_1 \int_0^{1-x_1} dx_2 \frac{1}{[x_1A+x_2B+(1-x_1-x_2)C]^3}, \\
&= -\int_0^1 dx_1 \int_0^{x_1} dx_2 \frac{1}{[x_1A+x_2B+(x_2-x_1)C]^3}, \\
&+ \int_0^1 dx_1 \int_0^1 dx_2 \frac{1}{[x_1A+x_2B+(x_2-x_1)C]^3}
\end{aligned}$$

Polylogarithms

Example

- Next one would like to perform these integrals. Some parameter integrals will be recognizable in terms of elementary functions and known special functions like Gauß's hypergeometric function. What remains are new iterated integrals that occur in field theory.
- After momentum integration the A, B and C will give scales that appear as parameters in these special functions.
- From this angle a Feynman diagram can be viewed as the problem of expressing the input in terms of known special functions and various iterated integrals. Simplifying, understanding and evaluating those iterated integrals is the topic of this talk.

Polylogarithms

Literature

The ‘earliest’ occurrence of a polylogarithm both in mathematics and particle physics is usually the dilogarithm,

$$\mathrm{Li}_2(x) = -\int_0^x dt \frac{\log(1-t)}{t} = -\int_0^x \frac{dt_1}{t_1} \int_0^{t_1} \frac{dt_2}{t_2 - 1}.$$

the first integral is for $z \in \mathbb{C}$ the second for $|z| < 1$. Notice that one might be tempted to define the dilogarithm as,

$$\int_0^x \frac{dt_1}{t_1} \int_0^{t_1} \frac{dt_2}{1 - t_2}.$$

Much is known about the dilogarithm. Below are just 2 example relations,

$$\mathrm{Li}_2(1) = \zeta(2), \qquad \mathrm{Li}_2(z) + \mathrm{Li}_2(-z) = \frac{1}{2}\mathrm{Li}_2(z^2).$$

Polylogarithms

Harmonic polylogarithms

Vermaseren and Remiddi defined the harmonic polylogarithms (HPLs),

$$f_1(x) = \frac{1}{1-x}, \qquad f_0(x) = \frac{1}{x}, \qquad f_{-1}(x) = \frac{1}{x+1},$$

which *violates* the convention choice made earlier. With these the harmonic polylogarithms are now defined,

$$H(\vec{a};x) := \int_0^x dt f_{a_1}(t) H(\vec{a}_{i>1};t), \quad H(\emptyset;x) = 1, \quad H(\vec{0};x) = \frac{1}{w!}\log^w x.$$

The length of $\vec{a} =: w$ is the weight of the polylogarithm. For example,

$$H(0,1;x) = \int_0^x dt \frac{H(1;t)}{t} = \int_0^x dt \frac{1}{t_1} \int_0^{t_1} dt_2 \frac{1}{1-t_2} = \mathrm{Li}_2(x).$$

Not all HPLs exist such as $H(1;1) = \log 0$.

Algebraic Relations

Properties

Harmonic polylogarithms enjoy several properties. The shuffle product $A \sqcup\!\sqcup B$ is the order preserving interlacing of two sets,

$$\{a, b\} \sqcup\!\sqcup \{c\} = \{\{a, b, c\}, \{a, c, b\}, \{c, a, b\}\}$$

then the harmonic polylogarithms satisfy,

$$H(\vec{a}; x)H(\vec{b}; x) = \sum_{\vec{c} \in \vec{a} \sqcup\!\sqcup \vec{b}} H(\vec{c}; x),$$

which are referred to as shuffle identities. Which is much clearer with an example,

$$\begin{aligned} H(0,1;x)H(1;x) &= H(0,1,1;x) + H(0,1,1;x) + H(1,0,1;x), \\ &= 2H(0,1,1;x) + H(1,0,1;x). \end{aligned}$$

Algebraic Relations

Properties

A second class of identities can be derived from integration by parts. One obtains the following general formula,

$$
\begin{aligned}
H(\vec{a};x) &= H(a_1;x)H(\vec{a}_{i>1};x) - \int_0^x dt f_{a_2}(t)H(a_1;t)H(\vec{a}_{i>2};t), \\
&= H(a_1;x)H(\vec{a}_{i>1};x) - H(a_2,a_1;x)H(\vec{a}_{i>2};x) + \cdots \\
&+ (-1)^{w+1}H(a_w,\ldots a_1;x).
\end{aligned}
$$

Again a simple example is,

$$
\begin{aligned}
H(1,1;x) &= H(1;x)H(1;x) - H(1,1;x), \\
\Rightarrow H(1,1;x) &= \frac{1}{2}H(1;x)^2.
\end{aligned}
$$

Algebraic Relations

Basis

Having such relations the natural task is to eliminate all algebraic relations and form a basis. (An algebraic relation is one involving positive integer powers of harmonic polylogarithms all evaluated at x and real coefficients.) There are $3^2 = 9$ weight 2 HPLs $\frac{3\times 2}{2}$ shuffle relations and 3 IBP relations so a weight 2 basis is,

$$H(0,1;x), \qquad H(-1,1;x), \qquad H(-1,0;x).$$

Some of the relations for the other weight 2 HPLs are,

$$H(1,-1;x) = H(-1;x)H(1;x) - H(-1,1;x),$$
$$H(0,0;x) = \frac{1}{2}H(0;x)^2.$$

For a review see for example the lecture notes by Ablinger & Blümlein '13 and references therein and for calculations Ablinger's HarmonicSums package.

Generalisations

Goncharov polylogarithm

More complicated Feynman diagrams lead one to observing complex letters which suggests to define the Goncharov polylogarithm,

$$G(\vec{a};x) := \int_0^x \frac{dt}{t-a_1} G(\vec{a}_{i>1};t), \qquad G(\emptyset;x) = 1, \qquad G(\vec{a};0) = 0,$$

for $a_i \in \mathbb{C}$. (Depending on $x \in \mathbb{C}$ it may be that there is a pole on the contour of integration this can be resolved but I will not discuss the topic.) Beyond the shuffle and integration by parts identities the Goncharov polylogarithm also has a scaling property,

$$G(\vec{a};x) = G(\alpha\vec{a};\alpha x),$$

for $\alpha \in \mathbb{C}$. (Beware trailing zeros!) Note however that there are minus signs when comparing an HPL to a Goncharov polylogarithm due to differing conventions,

$$G(0,1;x) = -H(0,1;x).$$

Generalisations

Hölder convolution

Goncharov polylogarithms also obey the Hölder convolution BORWEIN '01,

$$G(\vec{a};1) = \sum_{j=0}^{w} (-1)^j G(1-a_j, 1-a_{j-1}, \dots, 1-a_1; 1-p) G(a_{j+1}, \dots, a_w; p)$$

for $p \in \mathbb{C}$ arbitrary and $a_1 \neq 1$ and $a_w \neq 0$. Again an example cuts through the notation,

$$G(a,b;1) = G(\emptyset;1-p)\,G(a,b;p) - G(1-a;1-p)\,G(b;p) + G(1-b,1-a;1-p)\,G(\emptyset;p).$$

Relations of this type, depending on p are analytic; the argument changes and therefore are independent of how the basis was set-up. Thus one concludes that Goncharov polylogarithms satisfy (potentially) far more relations than the harmonic polylogarithm subset.

Generalisations

Multiple polylogarithms

There is yet another object of interest, the multiple polylogarithm, which is equivalent to the Goncharov polylogarithm but highlights some properties better.

$$\mathrm{Li}_{\vec{m}}(\vec{x}) = (-1)^w G\left(\vec{0}_{m_1-1}, \frac{1}{x_1}, \vec{0}_{m_2-1}, \frac{1}{x_1 x_2}, \ldots, \vec{0}_{m_w-1}, \frac{1}{\prod_{i=1}^{w} x_i}; 1\right)$$

and now w is the length of x or equivalently $\vec{m}$. Setting all arguments equal to one, $\vec{x} = \vec{1}$, gives the so-called multiple-ζ values,

$$\mathrm{Li}_{\vec{m}}(\vec{1}) = \zeta_{\vec{m}}.$$

In one dimension, $\vec{m} \in \mathbb{N}$, this further reduces to the usual Riemann ζ-function at natural arguments.

Generalisations

Stuffle relations

Multiple polylogarithms obey a stuffle relation which is quite involved to understand and I will omit. In short, rather than using a shuffle product to combine to lists of indices one uses a stuffle product. The relation is of the form,

$$\mathrm{Li}_{\vec{m}}(\vec{x})\mathrm{Li}_{\vec{n}}(\vec{y}) = \sum_i \mathrm{Li}_{\vec{r}_i}(\vec{s}_i),$$

the $\vec{r}_i$ and $\vec{s}_i$ come out of the stuffle product. An example for a little more clarity,

$$\mathrm{Li}_m(x)\mathrm{Li}_n(y) = \mathrm{Li}_{m,n}(x,y) + \mathrm{Li}_{n,m}(y,x) + \mathrm{Li}_{m+n}(xy)$$

One can of course translate this into the Goncharov notation. Stuffle relations are in addition to shuffle relations — not every GPL is an MPL!

Goncharov Conjecture

Basis redux

For a set of Goncharov polylogarithms there is the previous basis calculation where shuffle and integration by parts relations are removed. However, there are also the stuffle relations and the Hölder convolution plus the potential for unknown relations. This leads us into Goncharov's conjecture.

Conjecture

Any multiple polylogarithm beyond weight 1 may be expressed in terms of multiple polylogarithms without an index equal to 1.

This conjecture allows one to write down a handful of required functions. For example at weight 5 the conjecture implies only,

$$\mathrm{Li}_5(x), \quad \mathrm{Li}_{3,2}(x,y), \quad \mathrm{Li}_4(x), \quad \mathrm{Li}_{2,2}(x,y), \quad \mathrm{Li}_2(x), \quad \log(x).$$

are needed. While $\mathrm{Li}_{1,2}(x,y)$ is not needed for example.

Goncharov Conjecture

Computation

Let us perform this computation at weight 4 using the Mathematica package HarmonicSums. The start point is all possible weight 4 Goncharov polylogarithms; essentially one needs all possible ways of writing 4 different indices, 3 different indices, 2 different and finally a single index. After removing all shuffle and integration by parts relations there are 15 such polylogarithms which include,

$$G(a, b, c, d; 1), \qquad G(a, a, b, b; 1), \qquad G(a, b, b, b; 1).$$

Now it is possible to use two Hölder convolutions to 'insert a zero' into any polylogarithm without a zero index FRELLESVIG '16.

Goncharov Conjecture

Computation

Let us tackle a specific weight 2 example however the method is general. Given $G(a, b; x)$ $a, b \neq 0$ normalise the last index to 1,

$$G(a, b; x) = G\left(\frac{a}{b}, 1; \frac{x}{b}\right).$$

Compute a related Hölder convolution with $p = \frac{x}{b}$,

$$G\left(\frac{a}{b}, 1; 1\right) = -G\left(1; \frac{x}{b}\right) G\left(1 - \frac{a}{b}, 1 - \frac{x}{b}\right) + G\left(0, 1 - \frac{a}{b}, 1 - \frac{x}{b}\right) + G\left(\frac{a}{b}, 1; \frac{x}{b}\right)$$

Re-arranged for $G\left(\frac{a}{b}, 1; \frac{x}{b}\right)$ there is still a $w = 2$ polylogarithm without a zero index. Compute a second Hölder convolution now with $p = 0$,

$$G\left(\frac{a}{b}, 1; 1\right) = G\left(1 - \frac{a}{b}; 1\right) + G\left(0, 1 - \frac{a}{b}; 1\right).$$

Goncharov Conjecture

Computation

Combining the two Hölder convolution results allows one to write out that,

$$G(a,b;x) = G\left(1-\frac{a}{b};1\right) + G\left(0,1-\frac{a}{b};1\right) + G\left(1;\frac{x}{b}\right)G\left(1-\frac{a}{b},1-\frac{x}{b}\right) - G\left(0,1-\frac{a}{b},1-\frac{x}{b}\right).$$

Everything on the right-hand side is of lower weight or contains a zero. This procedure of computing two suitable Hölder convolutions in exact analogy to here always allows one to insert a zero into a non-zero index vector. Performing this to the weight 4 list of Goncharov polylogarithms and tidying up gets one down to the following list,

$$G(0,a,b,c;1), \quad G(0,0,a,b;1), \quad G(0,0,0,a;1), \quad G(0,a,0,b;1).$$

Goncharov Conjecture

Computation

Translating to the multiple polylogarithm notation the list contains,

$$\mathrm{Li}_{2,1,1}, \qquad \mathrm{Li}_{3,1}, \qquad \mathrm{Li}_{4}, \qquad \mathrm{Li}_{2,2}.$$

Now that we are in the multiple polylogarithm language one can apply the stuffle relations. Compute that,

$$\mathrm{Li}_3(x)\mathrm{Li}_1(y) = \mathrm{Li}_4(xy) + \mathrm{Li}_{1,3}(y,x) + \mathrm{Li}_{3,1}(x,y).$$

Now compute two shuffle relations,

$$\mathrm{Li}_1(x)\mathrm{Li}_3(xy) = \mathrm{Li}_{1,3}(y,x) + \mathrm{Li}_{2,2}(y,x) + \mathrm{Li}_{3,1}(y,x) + \mathrm{Li}_{3,1}(xy, \frac{1}{x}),$$
$$\mathrm{Li}_2(y)\mathrm{Li}_2(xy) = \mathrm{Li}_{2,2}(y,x) + \mathrm{Li}_{2,2}(xy, \frac{1}{x}) + 2\mathrm{Li}_{3,1}(y,x) + 2\mathrm{Li}_{3,1}(xy, \frac{1}{x}).$$

Goncharov Conjecture

Computation

One can solve these 3 relations to eliminate $\mathrm{Li}_{3,1}$ in favour of Li_4 and $\mathrm{Li}_{2,2}$ reducing us to the set,

$$\mathrm{Li}_{2,1,1}, \qquad \mathrm{Li}_4, \qquad \mathrm{Li}_{2,2}.$$

$\mathrm{Li}_{2,1,1}$ or equivalently $G(0,a,b,c;1)$ remains. I will not remove it because it is a problem outside computer algebra; there is no known algorithm to return an expression in terms of appropriate multiple polylogarithms. The result is known though FRELLESVIG '16.

Goncharov Conjecture

Computation

More generally this represents the current situation with regards to Goncharov's conjecture. It is possible, with existing algorithms to,

- return a small number of integrals that must be computed using analysis techniques or using some under appreciated combinations of known results.
- Explicitly verify the conjecture up to weight 4.
- Further relations, that help the conjecture may be found with numerics or intuition.

Using ideas of this type there is a library, CHAPLIN, which can evaluate harmonic polylogarithms in the complex plane Buehler & Duhr '11.

Numerics

Series

Having calculated Feynman diagrams and settled on a representation in terms of special functions the next issue is how to evaluate such expressions.

- A simple approach would be direct numerical integration however a better method is to find a rapidly converging series representation.

For $x \in (0,1)$ one may repeatedly apply a Maclaurin expansion to expand letters,

$$\frac{1}{x-a} = -\sum_{r=0}^{\infty} \frac{x^r}{a^{r+1}},$$

then integrate term by term to derive a sum for the whole polylogarithm. (Polylogarithms whose trailing index is zero do no directly admit such an expansion because of the $\log(x)$ which can not be expanded so one must extract this piece by shuffle products.)

Numerics

Series

Such a series will converge provided $\forall i \; |x| < |a_i|$. For HPLs the indices are $\{1, 0, -1\}$ so provided $|x| \ll 1$ the series is useful. For larger arguments one can use a variable transformation. In particular if,

$$x = \frac{1-t}{1+t} \quad \Rightarrow x \in (\sqrt{2}-1, 1) \Leftrightarrow t \in (0, \sqrt{2}-1).$$

Additionally by writing out an HPL,

$$H\left(\vec{a}; \frac{1-t}{1+t}\right) = \int_0^{\frac{1-t}{1+t}} d\tau f_{a_1}(\tau) H(\vec{a}_{i>1}; \tau),$$

then making successive variable transformations one can express the input in terms of HPLs at t. For example,

$$H\left(1; \frac{1-t}{1+t}\right) = -H(-1; 1) + H(-1; t) - H(0; t)$$

Everything on the left is at small argument so can be evaluated by a series representation.

Numerics

Bernoulli speed-up

For HPLs of arbitrary weight the above method suffices; series expansion for small argument then variable transformations to map from elsewhere on the complex plane to small argument HPLs.

- There is an additional speed-up option, the Bernoulli expansion, that helps with efficiency.
- At the innermost integral of any polylogarithm is a logarithm. The series expansion derived always contains an expansion of that logarithm.
- Better then is to write the expansion out in terms of logarithmic quantities.

Numerics

Bernoulli speed-up

Recall the dilogarithm definition,

$$\mathrm{Li}_2(x) = -\int_0^x dt \frac{\log(1-t)}{t} = \int_0^{-\log(1-x)} du \frac{u}{e^u - 1},$$
$$= \sum_{i=0}^{\infty} \frac{B_i}{(i+1)!}(-\log(1-x))^{i+1}.$$

This new expansion, using the Bernoulli numbers B_i, has much improved convergence because 'the logarithm is not expanded'.

Numerics

Bernoulli speed-up

This leads to whether one can apply the Bernoulli speed-up to HPLs? The answer is yes but there is a significant complication from the branch cut structure. Consider $H(-1,1;x)$ which contains branch cuts corresponding to both logarithms $\log(1-x)$ and $\log(1+x)$. To obtain a good series expansion one must separate out the polylogarithm into the two branch pieces,

$$H(-1,1;x) = \int_0^x dt \frac{H(1;t) - H(1;-1)}{t+1} + \int_0^x dt \frac{H(1;-1)}{t+1}$$

Separating the branch cut structure leads to a better behaved, and so faster, expansion.

Numerics

Bernoulli speed-up

One may recursively compute a separation of the HPL into two pieces with better analytic structure which can then be expanded using an appropriate logarithm. Avoiding a full discussion of this technicality one can write VOLLINGA '04,

$$H(\vec{a};x) = \sum_{i=0}^{\infty} \frac{C_{\vec{a}}(i)}{(i+1)!}(-\log(1-x))^{i+1}$$

where the C is quite a lot of work to compute,

$$C_{1,\vec{a}}(i) = \begin{cases} 0 & i = 0 \\ C_{\vec{a}}(i-1), & i > 0 \end{cases}, \quad C_{a_1+1,\vec{a}}(i) = \sum_{j=0}^{i} \binom{i}{j} \frac{B_{i-j}}{j+1} C_{a_1,\vec{a}}(j).$$

Numerics

Bernoulli speed-up

Then for a single index one uses,

$$C_1(i) = \delta_{0,i}, \qquad C_{n+1}(i) = \sum_{j=0}^{i} \binom{i}{j} \frac{B_{i-j}}{j+1} C_n(j).$$

There is another treatment in Gehrmann '01 where one considers the analytic structure of the HPLs and proceeds accordingly but it would be a technical summary of known ideas so the formulae are better here.
For a choice of basis up to weight 8 a FORTRAN library of the HPLs on $(0,1)$ is available Blümlein & MR.

Numerics

Goncharov Polylogarithm

Numerical evaluation of the Goncharov polylogarithm is significantly harder. Recall series convergence is poor when the argument is close to an index. With arbitrary complex indices allowed in general one can not always arrange to write a polylogarithm in a series that converges quickly. For example a variable transformation will generate new letters,

$$G\left(2; \frac{1-t}{1+t}\right) = G(-1; t) - G\left(-\frac{1}{3}; t\right) - G(0; 1) + G(0; 2).$$

The presence of $-\frac{1}{3}$ means variable transformations are not a general solution. Alternatively, one could return to the symbol and Goncharov's conjecture. Up to weight 4 it is possible to write out all Goncharov polylogarithms in terms of just a handful of functions of which only $\mathrm{Li}_{2,2}$ is not a well-known function. For an implementation see Frellesvig '16.

Numerics

GiNaC Recipe

In GiNaC there is another approach which can be slower but completely general Vollinga & Weinzierl '04.

- Recall our task is to write a given Goncharov polylogarithm in terms of polylogarithms with indices larger than the argument in magnitude.
- A sequence of variable transformations and integration by parts identities applied allows to write a series representation that converges.

A convergent series representation is delivered — it may converge slowly.

Numerics

GiNaC Recipe

A good implementation for experimental numerics would be a tabulation to fixed precision. If the series has no good convergence properties one can not be sure of how many terms to tabulate. The dangerous scenario is an index arbitrarily close to the argument,

$$a_i \simeq x.$$

Numerics

GiNaC Recipe

To speed-up convergence one can use the Hölder convolution. Recall $G(\vec{a}; x)$ converges poorly if there exists $a_i \simeq x$ with $|x| < |a_i|$. Normalise the polylogarithm of interest to have argument one then use the Hölder convolution with $p = \frac{1}{n}$ to write,

$$\begin{aligned} G(\vec{b}; 1) &= \sum_{j=0}^{w} (-1)^j G(1 - b_j, 1 - b_{j-1}, \ldots, 1 - b_1; \frac{1}{n}) G(b_{j+1}, \ldots, b_w; \frac{1}{n}), \\ &= \sum_{j=0}^{w} (-1)^j G(n - nb_j, n - nb_{j-1}, \ldots, n - nb_1; 1) \\ &\times G(nb_{j+1}, \ldots, nb_w; 1) \end{aligned}$$

with $\vec{b} = \vec{a}/x$. By assumption this converges so,

$$|b_j| > 1.$$

Numerics

GiNaC Recipe

After applying the Hölder convolution the convergence would be better if,

$$|nb_j| > |b_j| > 1 \Rightarrow n > 1, \quad |n(1-b_j)| = |n||1-b_j| > |1-b_j| > 0\#.$$

Thus one can not ensure that the polylogarithms in the Hölder convolution will converge. One must repeat the algorithm of transformations to express a polylogarithm in terms of convergent objects. Those objects that do converge, which includes the $j = 0$ term,

$$G(nb_1, \dots, nb_w; 1).$$

have improved convergence. Ultimately this procedure terminates and the resulting expression has improved convergence but GiNaC trades whether it is worth trying to improve convergence!

Numerics

In practice the problem is not yet fully solved;

- Current calculations run to weight 6 Goncharov polylogarithms and no minimal basis of functions is available.
- There can be sufficiently many polylogarithms to evaluate that efficiency is an issue. For example in $\bar{t}t$-production.

Better implementations can only occur by studying further and learning more.

Cyclotomic polylogarithms

Formalism

Our motivation for using the Goncharov polylogarithm is mathematical, physically quantities are real so it should be possible to find real representations of (at least some of) the Goncharov polylogarithms that occur in Feynman diagram calculations. These are the cyclotomic polylogarithms. The n^{th} cyclotomic polynomial is the unique factor free polynomial which divides $x^n - 1$ but no $x^k - 1$ for $k < n$.

$$\Phi_1(x) = x - 1, \qquad \Phi_2(x) = x + 1,$$
$$\Phi_3(x) = x^2 + x + 1, \qquad \Phi_4(x) = x^2 + 1,$$
$$\Phi_5(x) = x^4 + x^3 + x^2 + x + 1, \qquad \Phi_6(x) = x^2 - x - 1,$$

They are available in Mathematica using Cyclotomic[n,x].

Cyclotomic polylogarithms

Formalism

A cyclotomic polylogarithm is formed using letters,

$$f_k^l(x) = \frac{x^l}{\Phi_k(x)}.$$

Any polynomial of degree n has n roots in the complex plane so in principle one can factorise the cyclotomic polylogarithms and perform a partial fraction decomposition,

$$\Phi_6(x) = (-(-1)^{\frac{1}{3}} + x)((-1)^{\frac{2}{3}} + x)$$

$$\Rightarrow \frac{1}{\Phi_6(x)} = \frac{(-1)^{2/3}}{\left(1+\sqrt[3]{-1}\right)\left(x+(-1)^{2/3}\right)} + \frac{(-1)^{2/3}}{\left(1+\sqrt[3]{-1}\right)\left(\sqrt[3]{-1}-x\right)}.$$

This represents a general property; the cyclotomic polynomials factor into roots of unity. A cyclotomic polylogarithm is a Goncharov polylogarithm using only roots of unity and 0 for its indices.

Cyclotomic polylogarithms

Formalism

Issues concerning Goncharov polylogarithms are still to be resolved. Cyclotomic polylogarithms are far better behaved and understood. Immediately the convergence condition is satisfied for $x \in (0, 1)$,

$$|a_i| = 1 \Rightarrow |x_i| \leq |a_i|,$$

with a roughly constant convergence property for any cyclotomic polylogarithm. This means one can tabulate series and provide an efficient implementation. One is available to weight 4 and for cyclotomy 6 Blümlein & MR.

Cyclotomic polylogarithms

Constants

For large arguments one can use the same map as in the HPL case,

$$x = \frac{1-t}{1+t}.$$

Like before, constants are generated that refer to cyclotomic polynomials evaluated at 1. In the HPL case these numbers are well understood. For the Goncharov case little is known about these numbers and it is worth trying! This helps better understand possibly unknown relations. Pick a particular set of cyclotomic letters,

$$x, \quad f_1^0, \quad f_2^0, \quad f_3^1, \quad f_3^1, \quad f_4^0, \quad f_4^1, \quad f_6^0, \quad f_6^1.$$

Next generate all possible cyclotomic polylogarithms evaluated at one. (These are essentially Goncharov polylogarithms evaluated at up to 6^{th} roots of unity.)

Cyclotomic polylogarithms

Constants

Eliminate all shuffle, stuffle and integration by parts relations from these numbers meaning we have reduced to a basis. Additionally there is another set of relations, the distributive relations, which occur for polylogs at 1 with roots of unity indices Zhao '08.) Up to weight 4 one obtains,

weight	All	Basis
1	$1^9 = 9$	4
2	$2^9 = 81$	2
3	$3^9 = 729$	7
4	$4^9 = 6,561$	18

It remains to ask, could there be undiscovered relations Zhao '08?

PSLQ

We have seen many algebraic relations but hopefully there is still more to the story. To fully solve aspects of this issue one can perform numeric studies using the PSLQ algorithm.

PSLQ

Given a vector $\vec{v}$ construct when possible a $\vec{u} \in \mathbb{Z}^n$ with $|\vec{u}| \leq d$ such that $\vec{u} \cdot \vec{v} = 0$.

A simple example would be to use Mathematica's built-in function FindIntegerNullVector on $(\pi^2, \zeta(2))$. Mathematica returns,

$$\{1, -6\}.$$

Using GiNaC's evaluation tool one can evaluate the cyclotomic constants to some large number of digits, such as 10,000, then look for integer relations. PSLQ implementations allow one to control d which stops one finding relations with arbitrarily large coefficients.

PSLQ

Results

Broadhurst studied a problem of cyclotomic constants — cyclotomic polylogs at 1 — up to weight 3 and gave a set of numbers,

$$\pi, \quad \zeta(2), \quad \zeta(3), \quad \log(2), \quad \log(3), \quad \mathrm{Cl}_2\left(\frac{\pi}{3}\right) := \Im \mathrm{Li}_2(e^{\frac{i\pi}{3}}), \quad \mathrm{Li}_2\left(\frac{1}{4}\right),$$

plus the real and imaginary parts of,

$$\mathrm{Li}_3\left(\frac{e^{\frac{i\pi}{6}}}{2}\right), \qquad \mathrm{Li}_3\left(\frac{i}{\sqrt{3}}\right)$$

Recall that π and $\zeta(2)$ obey no PSLQ relation because $\zeta(2) \propto \pi^2$. Broadhurst and Bailey produced a FORTRAN PSLQ implementation (that is much better than Mathematica's). In principle one can write out vectors of various numbers and see whether for some d there are any relations amongst the numbers.

PSLQ
Literature

- A study of all Goncharov polylogarithms evaluated at the 6^{th}-roots of unity up to weight 6 was recently performed by Henn et al.
- We differ slightly from their treatment in that we come from a summation viewpoint and that means we consider a larger numbers of objects that close algebras of sums. (The sums are the Mellin transform of the cyclotomic polylogarithms.)

Additionally we are interested in proving results motivated by PSLQ to learn if there is really any reduction of polylogarithms that can help evaluation. There have been other analytic studies e.g. Kalmykov & Kniehl

PSLQ

Basis construction

The exercise we performed was a full basis construction. Namely,

- one computes all relations at weight 1 amongst the cyclotomic constants and the numbers Broadhurst gave.
- Then for weight 2, one computes all weight 2 numbers possible from a minimal set of the weight 1 numbers.
- Performs a PSLQ search to eliminate all relations between these elements and the weight 2 cyclotomic constants.

Continuing to weight 4 the results are,

Weight	All	Basis	PSLQ
1	$9^1 = 9$	4	4
2	$9^2 = 81$	2	2
3	$9^3 = 729$	7	5
4	$9^4 = 6,561$	18	10

for the cyclotomic polylogarithms at 1. (The same as Henn et al.)

PSLQ

Basis construction

A second exercise concerns the larger set of constants required to tabulate a numerical implementation of the cyclotomic polylogarithms to weight 4 with cyclotomy 6. These numbers originate from the,

$$x = \frac{1-t}{1+t}$$

transform and there are slightly more of them. They fully include the previous set. The results are,

Weight	Basis	New Numbers
1	5	1
2	8	3
3	41	14
4	185	< 40

The quantities of interest are in the form of real and imaginary parts; taking the numbers themselves there are only 155.

PSLQ
Relations

Most of these relations are checked to 10,000 digits while some later ones are new and are not verified to extremely high precision yet. Some example relations are ones missed by the basis construction. For example,

$$\frac{5}{4}\Im G(e^{-i\frac{\pi}{6}};1) = \Im G(e^{-i\frac{\pi}{3}};1) = -\frac{\pi}{3}.$$

This is an analytic relation not seen by the shuffle, stuffle, distributive and integration by parts identities. Or,

$$\Re G(e^{-i\frac{\pi}{6}}, e^{i\frac{5\pi}{6}};1) = -\frac{11}{288}\pi^2 - \frac{1}{2}\left[\Re G(e^{-i\frac{\pi}{6}};1)\right]^2 - 4\Re G(e^{-i\frac{5\pi}{6}}, e^{i\frac{\pi}{3}};1).$$

Proving theses relations from integral representations may be quite straightforward but one must know where to look.

Weight 1

At weights 1 and 2 one can expect to prove all relations using Lewin's monograph. The important point is that the treatment is now analytic; not algebraic. It is much harder to automate analytic procedures on a computer. For weight 1,

$$G(a;x) := \log\left(1 - \frac{x}{a}\right),$$

so it is easy to find results. The weight 1 6^{th} roots of unity (our conventions) lead to the following numbers,

$$\pi, \qquad \log(2), \qquad \log(3), \qquad \log(2-\sqrt{3}).$$

These numbers, and their higher weight generalisations, constitute a basis for other problems in field theory.

Weight 2

For weight 2 (it appears) everything is known. Roughly speaking the calculations proceed along the following lines. It is fairly easy to show that,

$$G(a,b;x) = \mathrm{Li}_2\left(\frac{b-x}{b-a}\right) - \mathrm{Li}_2\left(\frac{b}{b-a}\right) + \log\left(1-\frac{x}{b}\right)\log\left(\frac{x-a}{b-a}\right).$$

(In a region of the complex plane. Analytic continuation is possible with a careful treatment of branch cuts Moch et al. '02.

One can express the complex argument dilogarithm as,

$$\mathrm{Li}_2(re^{i\theta}) = \mathrm{Li}_2(r,\theta) + \omega\log(r) + \frac{1}{2}\mathrm{Cl}_2(2\omega) - \frac{1}{2}\mathrm{Cl}_2(2\theta+2\omega) + \frac{1}{2}\mathrm{Cl}_2(2\theta).$$

A classical result due to Kummer, see Lewin, with,

$$\omega := \tan^{-1}\left(\frac{r\sin\theta}{1-r\cos\theta}\right), \qquad \mathrm{Cl}_2(\theta) := -\int_0^\theta \log\left|2\sin\frac{x}{2}\right| dx.$$

Weight 2

Substituting in all the weight 2 cyclotomic polylogarithms and implementing all known special values of $\mathrm{Li}_2(r,\theta)$ one finds all the PSLQ relations and introduces additional new numbers,

$$\zeta(2), \quad \mathrm{Cl}_2\left(\frac{\pi}{6}\right), \quad \mathrm{Li}_2(\tfrac{1}{2}(\sqrt{3}-1)), \quad \Re[\mathrm{Li}_2(-\sqrt{\tfrac{2}{3}-\tfrac{1}{\sqrt{3}}}, \tfrac{5\pi}{12})],$$
$$\mathrm{Li}_2\left(\frac{1}{4}\right), \quad \log(\sqrt{3}-1), \quad \mathrm{Li}_2(\tfrac{1}{4}(3\sqrt{3}-5)), \quad \Re[\mathrm{Li}_2(\tfrac{\sqrt{\sqrt{3}+2}}{2}, \tfrac{\pi}{12})],$$
$$\mathrm{Cl}_2\left(\frac{\pi}{3}\right), \quad \mathrm{Li}_2(4\sqrt{3}-7), \quad \Re[\mathrm{Li}_2(-\tfrac{1}{\sqrt{2}}, \tfrac{5\pi}{12})], \quad \Im[\mathrm{Li}_2(\tfrac{\sqrt{2+\sqrt{3}}}{2}, \tfrac{\pi}{12})]$$

(PSLQ allows one to check there are no further relations amongst these numbers.) At weight 3 very little is known about the complex trilogarithm. As a result it is not possible to prove the PSLQ relations just by applying the literature and one starts to rely on the PSLQ results to introduce new transcendental numbers.

Summary

1. Today I have review the ongoing story of special functions in particle physics.
2. There are many relations and a lot known about polylogarithms but still there are open issues.
3. Fast numerical evaluation remains an issue for Goncharov polylogarithms.
4. There are still unstudied relations amongst polylogarithms and their particular values, essentially from weight 3 onwards.