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Johannes Bluemlein, Nikolai Fadeev, Carsten Schneider

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JOHANNES KEPLER UNIVERSITY LINZ Altenberger Str. 69 4040 Linz, Austria www.jku.at DVR 0093696

Computing Mellin representations and asymptotics of nested binomial sums in a symbolic way: the RICA package^{*}

Johannes Blümlein^a, Nikolai Fadeev^b, Carsten Schneider^b ^a Deutsches Elektronen-Synchrotron, DESY, 15738 Zeuthen, Germany ^b Research Institute for Symbolic Computation (RISC) Johannes Kepler University Linz, A-4040 Linz, Austria

Johannes.Bluemlein@desy.de,Nikolai.Fadeev@risc.jku.at,Carsten.Schneider@risc.jku.at

Abstract

Nested binomial sums form a particular class of sums that arise in the context of particle physics computations at higher orders in perturbation theory within QCD and QED, but that are also mathematically relevant, e.g., in combinatorics. We present the package RICA (Rule Induced Convolutions for Asymptotics), which aims at calculating Mellin representations and asymptotic expansions at infinity of those objects. These representations are of particular interest to perform analytic continuations of such sums.

The package RICA, which stands for Rule Induced Convolutions for Asymptotics, stem from the need to deal in a systematic way with finite and infinite nested binomial and inverse binomial sums that appear in the context of particle physics computations at higher orders in perturbation theory within QCD and QED [2]. This kind of analytic calculations of Feynman integrals, aim at high precision predictions for particle physics experiments for processes with massless partons but also massive quarks in QCD. They involve on the mathematical side the computation of increasingly complex iterated integrals. In the process of doing so, many different classes of functions arise, for example (generalized) harmonic sums and (generalized) harmonic polylogarithms [4]–[9]. The package HarmonicSums, developed by Jakob Ablinger [3], allows to manipulate efficiently such objects, and in particular find closed forms or simpler representations, compute (inverse) Mellin transforms, asymptotics, etc. thereof. Nevertheless, extensions of nested generalized harmonic sums weighted by the binomial coefficient $\binom{2n}{n}$ cannot be dealt with in the general case, and a different approach to treat them has been presented in [1]. Instead of relying on Mellin inversion through solving of differential equations [10], the method described in the former paper relies on recursive computations of Mellin convolutions of the summands of the iterated binomial sums. The main advantage of this approach is that by defining a set of possible general cases, i.e., classes of functions for which we can compute in general the Mellin inverse and/or the Mellin convolution, the computation of the Mellin inverse can be made rather fast and straightforward. Moreover, by identifying new general cases and adding them to our "dictionary", we can easily extend the classes of iterated sums we can deal with, even beyond the binomial case.

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Another advantage in representing the nested binomial sums as Mellin integrals is that one can perform asymptotic expansions at infinity, which helps us to obtain for example analytic continuations of those nested sums [1]. There exist several possible methods to perform asymptotic expansions of functions of the form $\int_0^1 dx \, x^n f(x)$, i.e., defined as Mellin transforms of some function f, depending on the regularity of f. In particular, there is a rather general method [11, 12] that relies on changes of variables and term by term integration [1], which has been implemented in the **RICA** package together with several variations or simpler methods to speed up computations.

Before presenting the main functions and an example of what our package can do, we want to emphasize the fact that while **RICA** implements and extends algorithms and methods that have not been implemented yet, it strongly relies on notations, objects and tools provided both by Carsten Schneider's **Sigma** package [13, 14] and Jakob Ablinger's **HarmonicSums** [3] package.

Let us define some notations, following [1]. We consider binomial nested sums, i.e. nested sum of the form:

$$BS(n) = \sum_{i_1=1}^n a_1(i_1; b_1, c_1, m_1) \sum_{i_2=1}^n a_2(i_2; b_2, c_2, m_2) \cdots \sum_{i_k=1}^n a_k(i_k; b_k, c_k, m_k)$$

where $a_p(i; b, c, m) = {\binom{2i}{i}}^{b} \frac{c^i}{i^m}$, $b \in \{-1, 0, 1\}$, $c \in \mathbb{R}^*$, $m \in \mathbb{N}$, and almost all of the *b* are 0 except for some that fit into the case of the theorems described in [1, Section 4]. We also accept coefficients that have a more general structure, such as $\frac{c^i}{2i+1} {\binom{2i}{i}}^{b}$, $b \in \{-1, 1\}$, that we extended to cases of the form $\frac{p(i)}{q(i)} {\binom{2i}{i}}$, where $p, q \in \mathbb{C}[X]$, deg $p \leq \deg q$.¹

Now we present the main functionalities of our package. Once installed, we have to load it in Mathematica:

$\ln[1] := << {\rm RICA.m};$

Rule Induced Convolutions for Asymptotics (RICA) package by Nikolai Fadeev © RISC-JKU

As stated before, **RICA** depends on **Sigma** and **HarmonicSums** which have to be loaded beforehand. The three main functions of the package are the following:

• SumToMellin[expr,c,x,opts]: Given an argument expr that is a linear combination of binomial nested sums, it computes its Mellin inverse. More precisely, the argument expr has the following form:

$$\exp r = \sum_{i=1}^{m} \alpha_i \operatorname{GS}\left[\{f_{i,1}(\operatorname{VarGL}), f_{i,2}(\operatorname{VarGL}), \dots, f_{i,p_i}(\operatorname{VarGL})\}, n\right], \alpha_i \in \mathbb{C}, \ p_i \in \mathbb{N}$$

and GS is the generalized iterated sum defined in HarmonicSums as

$$\operatorname{GS}\left[\{f_1(\operatorname{VarGL}), f_2(\operatorname{VarGL}), \dots, f_p(\operatorname{VarGL})\}, n\right] = \sum_{1 \le i_p \le i_{p-1} \le \dots \le i_1 \le n} f_1(i_1) f_2(i_2) \cdots f_p(i_p).$$

The second argument c specifies a variable that is used to denote the constants that might appear in the final expression², and x is the integration variable in the Mellin integrals.

¹Currently we are working on extensions that cover any rational function and more complicated coefficients. ²In particular if we give for example C, the constants will be denoted as C_i .

Finally, opts is an optional boolean argument called ToGLbBasis which uses HarmonicSums basis reduction functions to simplify the result further; its default value is True.

The output is returned in the form of a tuple where the first element is a linear combination of Mellin transforms, using HarmonicSums notation Mellin $[k_n(x), f(x)] = \int_0^1 dx \, k_n(x) f(x)$ where $k_n(x) = (ax)^n$ or $k_n(x) = (ax)^n - 1$ is the kernel, i.e.

$$\exp r = \sum_{i=1}^{p} \alpha_i \operatorname{Mellin}[k_{i,n}(x), f_i(x)]$$

The second element is then a list of the values of those constants, i.e.,

$$\{C_1 \rightarrow \text{value}_1, \dots, C_p \rightarrow \text{value}_p\}$$

that might arise inside of the functions $f_i(x)$.

• AsymptoticsMellint[expr, x, n, ord, opts]: This function computes the asymptotic expansion of a linear combination of Mellin integrals. It takes as the main argument expr which is a linear combination of Mellin representations as obtained in the output of SumToMellin, together with x which is the Mellin integration variable, n which is the Mellin parameter, ord which is the required order of the expansion, and opts which allows to insert possible fine-tuning options.

The output is returned as an asymptotic expansion similar to what Mathematica does when using the built-in function Series.

• AsymptoticsSum[expr,n,x,ord]: The function can be seen as a "combination" of both functions above, i.e. "AsymptoticsSums = AsymptoticsMellint \circ SumToMellin". It takes therefore as the main argument expr, i.e. a linear combination of nested binomial sums in the GS representation, together with the Mellin parameter n, Mellin integration variable x and desired expansion order ord.

The output is in the same form as AsymptoticsMellint.

To conclude, below is an explicit example of a computation using all functions above. We consider the nested binomial sum:

$$S(n) = \sum_{i=1}^{n} \frac{1}{i\binom{2i}{i}} \sum_{j=1}^{i} (-2)^{j}\binom{2j}{j} = GS\left[\left\{\frac{1}{\operatorname{VarGL}\binom{2\operatorname{VarGL}}{\operatorname{VarGL}}}, (-2)^{\operatorname{VarGL}\binom{2\operatorname{VarGL}}{\operatorname{VarGL}}}\right\}, n\right]$$

by introducing it in Mathematica as follows:

 $In[2]:= sum1 = GS\left[\left\{\frac{1}{VarGL * Binomial(2VarGL, VarGL)}, (-2)^{VarGL} * Binomial(2VarGL, VarGL)\right\}, n\right];$ Now we apply SumToMellin to the input expression and get:

ln[3] = mel1 = SumToMellin[sum1, C, x]

$${}_{Out[3]=} \left\{ \text{Mellin}\left[(-2)^n x^n - 1, \frac{1 - \frac{1}{6\sqrt{2}\sqrt{x + \frac{1}{6}}}}{x + \frac{1}{2}} \right] - \frac{2}{3} \text{Mellin}\left[4^{-n} x^n - 1, \frac{1}{\sqrt{1 - x}(x - 4)} \right], \{\} \right\}$$

As we see, the result is a sum of two Mellin integral representations where no extra constants arise. We are now in the position to apply the function AsymptoticsMellint to get the asymptotic expansion, e.g., up to order 4:

In[4]:= AsymptoticsMellint[mel1[[1]], x, n, 7]

Out[4]= -	$26425(-1)^n 2^{n+3}$	$2213(-1)^{n}2^{n+3}$	$799(-1)^{n}2^{n+3}$	$73(-1)^{n}2^{n+3}$	$5(-1)^{n}2^{n+3}$	$7(-1)^{n}2^{n+3}$	$(-1)^{n}2^{n+4}$
	531441n ⁷		59049n ⁵	6561n ⁴	729n ³	243n ²	27n

Using the function AsymptoticsSum, if we only wanted the asymptotic expansion and not the Mellin representation we could have simply called it directly:

ln[5]:= AsymptoticsSum[sum1, n, x, 7]

Out[5]= -	$26425(-1)^{n}2^{n+3}$	$2213(-1)^n 2^{n+3}$	$799(-1)^{n}2^{n+3}$	$73(-1)^{n}2^{n+3}$	$5(-1)^{n}2^{n+3}$	$7(-1)^{n}2^{n+3}$	$(-1)^{n}2^{n+4}$
	531441n ⁷	$-177147n^{6}$	59049n ⁵	6561n ⁴	729n ³	243n ²	27n

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