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

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Different problems in combinatorics, analysis of algorithms or even physics involve binomially weighted sums

Example 1 (combinatorics): In the paper [Evaluation of Binomial Double Sums Involving Absolute Values of C. Krattenthaler and C. Schneider], sums of the following form appear for the study of double sums with binomial coefficients:

$$-2^{2m+1}n\binom{2n}{n}\sum_{i=0}^{m}\frac{2^{-2i\binom{2i}{i}}}{i+n}+2\binom{2m}{m}\binom{2n}{n}+2^{2m+2n}$$

If we want the asymptotic expansion at  $m\to+\infty$  for fixed m, this involves in particular computing the asymptotics of the boxed sum

**Motivation** Notation

**Example 2 (physics)**: Particle physics computations are often done in Mellin space, and for example in the paper  $[The O(\alpha_s^3 T_F^2) \text{ contributions to the gluonic operator matrix element by J.Abligner, J. Blümlein, C. Schneider et al.], sums of the following form pop up:$ 

$$\frac{1}{4^n} \binom{2n}{n} \left( \sum_{i=1}^n \frac{4^i}{i^2 \binom{2i}{i}} S_1(i-1) \right) - 7\zeta_3 \right), \quad S_1(i-1) := \sum_{k=1}^{i-1} \frac{1}{k}, \quad \zeta_k = \sum_{n=1}^\infty \frac{1}{n^k}$$

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Sums can be nested, for example in [Iterated Binomial Sums and their Associated Iterated Integrals by J.Ablinger, J.Blümlein, C.G. Raab and C. Schneider], we also have sums such as:

$$\sum_{i=1}^{n} \binom{2i}{i} S_2(i), \quad \sum_{i=1}^{n} \frac{1}{i\binom{2i}{i}} \sum_{j=1}^{i} \binom{2j}{j} (-2)^j$$

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**Aim**: Being able to deal automatically with those kind of sums in all generality, in particular **Mellin inversion** and **asymptotic expansion** 

We define the binomially weighted sums as follows:

$$BS_{\{a_1,\dots,a_k\}}(n) := \sum_{i_1=1}^n a_1(i_1) \sum_{i_2=1}^{i_1} a_2(i_2) \cdots \sum_{i_k=1}^{i_{k-1}} a_k(i_k)$$

with

$$a_j(p) = a_j(p; b, c, m) = {\binom{2p}{p}}^b \frac{c^p}{p^m}, \quad b \in \{-1, 0, 1\}, \ c \in \mathbb{R}^*, \ m \in \mathbb{N}$$

[Harmonic Sums, Mellin transforms and integrals by J.A.M. Vermaseren]

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Example: 
$$\sum_{i=1}^{n} \frac{1}{i\binom{2i}{i}} \sum_{j=1}^{i} \binom{2j}{j} \frac{(-1)^{j}}{j^{3}} \sum_{k=1}^{j} \frac{\left(\frac{1}{2}\right)^{k}}{k^{2}}$$

[Harmonic Sums, Mellin transforms and integrals by J.A.M. Vermaseren]

More generic summands can also be considered, such as:

$$\frac{c^n}{(2n+1)\binom{2n}{n}} \text{ or } \frac{p(i)}{q(i)}\binom{2i}{i}, \ p,q \in \mathbb{C}[X], \ \deg p \leq \deg q, \ \operatorname{roots}(q) \subset \mathbb{C} \backslash \mathbb{R}_+$$

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Example : 
$$\sum_{i=1}^n \frac{1+i}{i^2+5i+6} \sum_{j=1}^i \frac{(-2)^j}{(2j+1)\binom{2j}{j}} \sum_{k=1}^j \frac{3^k}{k^2}$$

[Harmonic Sums, Mellin transforms and integrals by J.A.M. Vermaseren]

We remind here some definitions and useful properties of Mellin transforms:

Definition:

$$M[f(x)](n) := \int_0^1 \mathrm{d}x \, x^n f(x)$$

Summation formula ( $c \in \mathbb{C}$ ):

$$\sum_{i=1}^{n} c^{i} M\left[f(x)\right](i) = c^{n} M\left[\frac{x}{x-\frac{1}{c}}f(x)\right](n) - M\left[\frac{x}{x-\frac{1}{c}}f(x)\right](0) \quad (1)$$

Convolution:

$$f(x) * g(x) := \int_0^1 \mathrm{d}x_1 \, \int_0^1 \mathrm{d}x_2 \, \delta(x - x_1 x_2) f(x_1) g(x_2) = \int_x^1 \mathrm{d}y \, \frac{f(y)}{y} g\left(\frac{x}{y}\right)$$
$$M\left[f(x) * g(x)\right](n) = M\left[f(x)\right](n) \cdot M\left[g(x)\right](n)$$

#### Question: How to represent them as Mellin integrals?



▶ First method (used by HarmonicSums for general Mellin inversion): given *M* [*f*(*x*)] (*n*) as holonomic sequences, we obtain the associated holonomic differential equation, and by solving it we can obtain a closed form for *f*(*x*)



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Second method: compute it recursively from the BS using fundamental properties of Mellin transforms and "rule-theorems" that allow us to compute in an automatic way Mellin convolutions [Iterated Binomial Sums and their

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Note: RICA relies on C. Schneider's Sigma and J. Ablinger's HarmonicSums

Note: These Mellin representations will involve general polylogarithms

$$\mathrm{H}^*_{\emptyset}(x):=1, \ \mathrm{H}^*_{\mathrm{b}(\mathrm{t}),\overrightarrow{c}\,(\mathrm{t})}(x)=\mathrm{H}^*_{\mathrm{b},\overrightarrow{c}}(x):=\int_x^1\mathrm{d}t\,b(t)\mathrm{H}^*_{\overrightarrow{c}}(t)$$

Defined over a 37 letter alphabet  $\{f_0, \ldots, f_{w_{32}}\}$  containing root singularities such that all iterated integrals are linearly independent over the algebraic functions, and obeying shuffle algebra

[Harmonic polylogarithms by E. Remiddi and J.A.M. Vermaseren]

[Harmonic Sums and Polylogarithms Generated by Cyclotomic Polynomials by J. Ablinger, J. Blümlein and C. Schneider] [Iterated Binomial Sums and their Associated Iterated Integrals by J. Ablinger, J. Blümlein, C.G. Raab and C. Schneider]

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#### Example:

$$\begin{aligned} \mathbf{H}_{\mathbf{f}_{w_{11}},\mathbf{f}_{2},\mathbf{f}_{w_{8}}}^{*} &= \int_{x}^{1} \mathrm{d}t_{1} \, f_{w_{11}}(t_{1}) \int_{t_{1}}^{1} \mathrm{d}t_{2} \, f_{2}(t_{2}) \int_{t_{2}}^{1} \mathrm{d}t_{3} \, f_{w_{8}}(t_{3}) \\ &= \int_{x}^{1} \mathrm{d}t_{1} \, \frac{1}{t_{1}\sqrt{1-t_{1}}\sqrt{2-t_{1}}} \int_{t_{1}}^{1} \mathrm{d}t_{2} \, \frac{1}{2-t_{2}} \int_{t_{2}}^{1} \mathrm{d}t_{3} \, \frac{1}{t_{3}\sqrt{t_{3}-\frac{1}{4}}} \end{aligned}$$

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Example: (linearization by shuffle relations)

$$\mathbf{H}^{*}_{\mathbf{f}_{1}}(x)\mathbf{H}^{*}_{\mathbf{f}_{0},\mathbf{f}_{-1}}(x) = \mathbf{H}^{*}_{\mathbf{f}_{1},\mathbf{f}_{0},\mathbf{f}_{-1}}(x) + \mathbf{H}^{*}_{\mathbf{f}_{0},\mathbf{f}_{-1},\mathbf{f}_{1}}(x) + \mathbf{H}^{*}_{\mathbf{f}_{0},\mathbf{f}_{1},\mathbf{f}_{-1}}(x)$$

where

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

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#### Example:

$$BS(n) = \sum_{k=1}^{n} {\binom{2i}{i}} S_2(i) = \sum_{k=1}^{n} {\binom{2i}{i}} \sum_{j=1}^{i} \frac{1}{i^2}$$

First we compute the Mellin representation of  $\frac{1}{i^2}$  by convolving  $\frac{1}{i} = M\left[\frac{1}{x}\right](i)$  with itself. We get:

$$\frac{1}{i^2} = M\left[\frac{1}{x}\right](i) \cdot M\left[\frac{1}{x}\right](i) = M\left[\frac{1}{x} * \frac{1}{x}\right](i) = M\left[\frac{\mathrm{H}_0^*(x)}{x}\right](i)$$

where

$$H_0^*(x) := \int_x^1 dt \, f_0(t) = \int_x^1 dt \, \frac{1}{t} = -\log x$$

Using the summation formula (1), we can then obtain:

$$S_{2}(i) = \sum_{k=1}^{i} M\left[\frac{\mathrm{H}_{0}^{*}(x)}{x}\right](i) = \underbrace{\int_{0}^{1} \mathrm{d}x \, x^{i} \frac{\mathrm{H}_{0}^{*}(x)}{x-1}}_{M\left[\frac{x}{x-1} \frac{\mathrm{H}_{0}^{*}(x)}{x}\right](i)} - \underbrace{\int_{0}^{1} \mathrm{d}x \, \frac{\mathrm{H}_{0}^{*}(x)}{x-1}}_{M\left[\frac{x}{x-1} \frac{\mathrm{H}_{0}^{*}(x)}{x}\right](i)} = \int_{0}^{1} \mathrm{d}x \, x^{i} \frac{\mathrm{H}_{0}^{*}(x)}{x-1} + \zeta_{2}$$

where

$$\zeta_2 = \sum_{i=1}^{\infty} \frac{1}{i^2} = \frac{\pi^2}{6}$$

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Now that the innermost sum has as integral representation, we shift to the next and last level. First, one can show (e.g. direct integration) that:

$$\binom{2i}{i} = \frac{4^i}{\pi} M \left[ \frac{1}{\sqrt{x(1-x)}} \right] (i)$$

So that

$$\sum_{i=1}^{k} \binom{2i}{i} S_2(i) = \frac{1}{\pi} \sum_{i=1}^{n} 4^i M \left[ \frac{1}{\sqrt{x(1-x)}} \right] (i) \cdot M \left[ \frac{\mathrm{H}_0^*(x)}{x-1} \right] (i) + \frac{\zeta_2}{\pi} \sum_{i=1}^{k} 4^i M \left[ \frac{1}{\sqrt{x(1-x)}} \right] (i)$$

• We apply again the summation formula to obtain first the second part:

$$\frac{\zeta_2}{\pi} \sum_{i=1}^k 4^i M\left[\frac{1}{\sqrt{x(1-x)}}\right](i) = \frac{\zeta_2}{\pi} \int_0^1 \mathrm{d}x \, \frac{(4x)^n - 1}{x - \frac{1}{4}} \sqrt{\frac{x}{1-x}}$$

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Then we switch to the first part of the binomial and convolve the functions:

$$M\left[\frac{1}{\sqrt{x(1-x)}}\right](i) \cdot M\left[\frac{\mathrm{H}_{0}^{*}(x)}{x-1}\right](i) = M\left[\int_{x}^{1} \mathrm{d}y \, \frac{\mathrm{H}_{0}^{*}(y)}{(y-1)\sqrt{y-x}}\right](i)$$

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A set of several "rule-theorems" have been proven in [Iterated Binomial Sums and their Associated Iterated Integrals by J. Ablinger, J. Blümlein, C.G. Raab and C. Schneider] to simplify further such expressions. One of them allows us to get:

$$\int_{x}^{1} \mathrm{d}y \, \frac{\mathrm{H}_{0}^{*}(y)}{(y-1)\sqrt{y-x}} = \frac{\mathrm{H}_{\mathrm{b},\mathrm{w}_{1}}^{*}(x)}{\sqrt{x-1}}, \ f_{b}(x) = \frac{1}{\sqrt{x(x-1)}}, \ f_{w_{1}}(x) = \frac{1}{\sqrt{x(1-x)}}$$

Using the shuffle algebra, we can reduce the expression down to:

$$M\left[\frac{\mathbf{H}_{\mathbf{b},\mathbf{w}_{1}}^{*}(x)}{\sqrt{x(x-1)}}\right](i) = -M\left[\frac{\mathbf{H}_{\mathbf{w}_{1}}^{*}(x)^{2}}{2\sqrt{x(1-x)}}\right](i)$$

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Finally, using once again the summation formula we get:

$$\sum_{i=1}^{n} 4^{i} M\left[\frac{\mathrm{H}_{\mathrm{w}_{1}}^{*}(x)^{2}}{2\sqrt{x(1-x)}}\right](i) = \int_{0}^{1} \mathrm{d}x \, \frac{(4x)^{n} - 1}{x - \frac{1}{4}} \sqrt{\frac{x}{1-x}} \frac{\mathrm{H}_{\mathrm{w}_{1}}^{*}(x)^{2}}{2}$$

and resumming everything, we get:

$$\sum_{i=1}^{n} \binom{2i}{i} S_2(i) = -\frac{1}{\pi} \int_0^1 \mathrm{d}x \, \frac{(4x)^n - 1}{x - \frac{1}{4}} \sqrt{\frac{x}{1 - x}} \left( \frac{\mathrm{H}_{w_1}^*(x)^2}{2} - \zeta_2 \right)$$

We now want to obtain an asymptotic expansion for  $n \to +\infty$  up to order p of a general expression of the form:

$$\tilde{M}_{a}[f(x)](n) := \int_{0}^{1} \mathrm{d}x \, \frac{(ax)^{n} - 1}{x - \frac{1}{a}} f(x) = \int_{0}^{1} \mathrm{d}x \, [(ax)^{n} - 1] \, \tilde{f}(x) \tag{2}$$

where

$$\tilde{f}(x) := \frac{f(x)}{x - \frac{1}{a}}$$

- There exist several method to compute this expansion, depending mostly on the regularity of f and whether the integral can be split [*terated Binomial Sums and their Associated Iterated Integrals* by J. Ablinger, J. Blümlein, C.G. Raab and C. Schneider]
- We will present one of the methods, all of them are implemented in RICA

We suppose that f is regular on [0;1] and a < -1, so that  $\frac{1}{x-\frac{1}{a}}$  is regular on [0;1] and we can simply split the integral in two, then use a **change of variables** 

Split the Mellin integral, factor out the a<sup>n</sup>:

$$\int_0^1 \mathrm{d}x \, \frac{ax^n - 1}{x - \frac{1}{a}} f(x) = a^n M\left[\frac{f(x)}{x - \frac{1}{a}}\right](n) - \underbrace{M\left[\frac{f(x)}{x - \frac{1}{a}}\right](0)}_{=:C}$$

**Note**: When |a| > 1, the constant C is exponentially suppressed

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**Note**: When |a| > 1, the constant C is exponentially suppressed In  $M\left[\frac{f(x)}{x-\frac{1}{a}}\right](n)$ , we make the following change of variables:

$$x = e^{-z}, \quad \mathrm{d}x = -e^{-z}\mathrm{d}z$$

and end up with:

$$M\left[\frac{f(x)}{x-\frac{1}{a}}\right](n) = a^n \int_0^{+\infty} dz \, e^{-zn} \underbrace{\frac{e^{-z}}{e^{-z}-1} f(e^{-z})}_{=:g(z)}$$

Setting
Mellin inversion
Asymptotic expansions
Mathematica session

• We expand g(z) around z = 0 up to the order p:

$$g(z) \underset{z \to 0}{=} \sum_{\alpha \le p} g_{\alpha} z^{\alpha} + \mathcal{O}(z^{\alpha+1}), \quad \alpha \in \frac{1}{2} \mathbb{Z}_{\ge -1}, \ g_{\alpha} \in \mathbb{R}$$

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Finally we integrate  $M[\frac{f(x)}{x-\frac{1}{a}}](n)$  using the expansion above, and adding the  $a^n$  coefficient back:

$$\tilde{M}_{a}[f(x)](n) =_{n \to +\infty} a^{n} \sum_{\alpha \le p} \int_{0}^{+\infty} dz \, e^{-zn} g_{\alpha} z^{\alpha}$$
$$= a^{n} \sum_{\alpha \le p} \frac{h_{\alpha}}{n^{\alpha}}, \quad h_{\alpha} \in \mathbb{R}$$

First we preload Sigma and HarmonicSums:

 $\ln[1] = << {\bf Sigma.m};$ 

Sigma - A summation package by Carsten Schneider - © RISC

ln[2] = << HarmonicSums.m;

HarmonicSums by Jakob Ablinger – © RISC

And then our package:

ln[3] := << RICA.m;

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

First we preload Sigma and HarmonicSums:

 $ln[6] = \langle \mathbf{Sigma.m};$ 

Sigma - A summation package by Carsten Schneider - © RISC

ln[7] = << HarmonicSums.m;

HarmonicSums by Jakob Ablinger - © RISC

And then our package:

ln[8] := << RICA.m;

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

We define the sum that we want to study using HarmonicSums' GS function:  $In[9]:= \mathbf{sum1} = \mathbf{GS} \left[ \left\{ \mathsf{Binomial}[2 \; \mathsf{VarGL}, \mathsf{VarGL}], \frac{1}{\mathsf{VarGL}^2} \right\}, n \right];$ 

First we preload Sigma and HarmonicSums:

 $\ln[11] = << {\bf Sigma.m};$ 

Sigma - A summation package by Carsten Schneider - © RISC

ln[12] = << HarmonicSums.m;

HarmonicSums by Jakob Ablinger – © RISC

And then our package:

ln[13] = << RICA.m;

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

We define the sum that we want to study using HarmonicSums' GS function:  $In[14]:= \mathbf{sum1} = \mathbf{GS} \left[ \left\{ Binomial[2 VarGL, VarGL], \frac{1}{VarGL^2} \right\}, \mathbf{n} \right];$ 

We can now compute the Mellin representation:

ln[15] = mel1 = SumToMellin[sum1, C, x]

$$Out[15]= \left\{-\frac{2\mathsf{Mellin}\left(4^nx^n-1,\frac{\sqrt{x}(\mathsf{Hwb}[\{\mathsf{fw1}\},x]^2-2z2)}{\sqrt{1-x}(4x-1)}\right)}{\pi},\{\}\right\}$$



We can now compute the asymptotics, either from the Mellin representation...

 $\label{eq:lin_lin} \ensuremath{\mathsf{ln}}{\sc 16}{\sc :=} \ensuremath{\operatorname{asymptoticsMellint}}{\sc 16}{\sc 16}{\sc$ 

Out[16]=

$$-\frac{2}{\pi} \left( -\frac{(\pi-12)(12+\pi)\sqrt{\pi}2^{2n-3}}{27n^{3/2}} - \frac{\left(288+59\pi^2\right)\sqrt{\pi}2^{2n-7}}{27n^{5/2}} - \frac{97\left(25\pi^2-432\right)\sqrt{\pi}2^{2n-10}}{81n^{7/2}} - \frac{17\left(33929\pi^2-440640\right)\sqrt{\pi}2^{2n-15}}{243n^{9/2}} - \frac{\pi^{5/2}2^{2n}}{9\sqrt{n}} \right)$$



We can now compute the asymptotics, either from the Mellin representation...

 $\label{eq:ln[17]:=asymp1 = AsymptoticsMellint[mel1[[1]], x, n, 4]} \\ \\$ 

$$-\frac{2}{\pi} \left( -\frac{(\pi-12)(12+\pi)\sqrt{\pi}2^{2n-3}}{27n^{3/2}} - \frac{\left(288+59\pi^2\right)\sqrt{\pi}2^{2n-7}}{27n^{5/2}} - \frac{97\left(25\pi^2-432\right)\sqrt{\pi}2^{2n-10}}{81n^{7/2}} - \frac{17\left(33929\pi^2-440640\right)\sqrt{\pi}2^{2n-15}}{243n^{9/2}} - \frac{\pi^{5/2}2^{2n}}{9\sqrt{n}} \right)$$

... or directly from the sum representation:

ln[18] = asymptoticsSum[sum1, n, x, 3]

$$\begin{array}{l} \text{Out}[18]= & -\frac{2}{\pi} \left( -\frac{(\pi-12)(12+\pi)\sqrt{\pi}2^{2n-3}}{27n^{3/2}} - \frac{\left(288+59\pi^2\right)\sqrt{\pi}2^{2n-7}}{27n^{5/2}} - \frac{97 \left(25\pi^2-432\right)\sqrt{\pi}2^{2n-10}}{81n^{7/2}} \right. \\ & \left. -\frac{17 \left(33929\pi^2-440640\right)\sqrt{\pi}2^{2n-15}}{243n^{9/2}} - \frac{\pi^{5/2}2^{2n}}{9\sqrt{n}} \right) \end{array}$$



We can now compute the asymptotics, either from the Mellin representation...

 $\label{eq:lins} \ensuremath{\mathsf{ln}}\xspace{19]:=} asymptoticsMellint[mel1[[1]], x, n, 4]$ 

$$\begin{array}{l} \text{Out}[19]=\\ &-\frac{2}{\pi}\left(-\frac{(\pi-12)(12+\pi)\sqrt{\pi}2^{2n-3}}{27n^{3/2}}-\frac{\left(288+59\pi^2\right)\sqrt{\pi}2^{2n-7}}{27n^{5/2}}-\frac{97\left(25\pi^2-432\right)\sqrt{\pi}2^{2n-10}}{81n^{7/2}}\right.\\ &-\frac{17\left(33929\pi^2-440640\right)\sqrt{\pi}2^{2n-15}}{243n^{9/2}}-\frac{\pi^{5/2}2^{2n}}{9\sqrt{n}}\right)\\ \text{In}[20]:=\text{DiscretePlot}\left[\frac{|\text{sum1}-\text{asymp1}|}{|\text{sum1}|},\{\text{n},1,50\}\right]\\ \text{Out}[10] \end{array}$$

Out[20]=



Here's another example:

$$\label{eq:lin21:=sum2} \mbox{In[21]:= sum2} = \mathbf{GS} \left[ \left\{ (-2)^{\mbox{VarGL}} \mbox{Binomial[2VarGL, VarGL]}, \frac{\left(\frac{1}{2}\right)^{\mbox{VarGL}}}{\mbox{VarGL}}, \frac{1}{\mbox{VarGL}^2} \right\}, \mathbf{n} \right];$$

Setting Mellin inversion Asymptotic expansions Mathematica session

Here's another example:

$$\label{eq:linear} \mbox{In[22]:= sum2 = GS} \left[ \left\{ (-2)^{\mbox{VarGL}} \mbox{Binomial[2VarGL, VarGL]}, \frac{\left(\frac{1}{2}\right)^{\mbox{VarGL}}}{\mbox{VarGL}}, \frac{1}{\mbox{VarGL}^2} \right\}, n \right];$$

 $\label{eq:ln[23]:=} In[23]:= ToHarmonicSumsSum[sum2]$ 

$$\operatorname{Out}[23]= \sum_{\tau_1=1}^{n} (-2)^{\tau_1} \operatorname{Binomial}[2\tau_1, \tau_1] \left( \sum_{\tau_2=1}^{\tau_1} \frac{2^{-\tau_2} \left( \sum_{\tau_3=1}^{\tau_2} \frac{1}{\tau_3^2} \right)}{\tau_2} \right)$$



Here's another example:

$$\label{eq:In[24]:=} \mbox{sum2} = \mathbf{GS} \left[ \left\{ (-2)^{\mbox{VarGL}} \mbox{Binomial}[2\mbox{VarGL},\mbox{VarGL}], \frac{\left(\frac{1}{2}\right)^{\mbox{VarGL}}}{\mbox{VarGL}}, \frac{1}{\mbox{VarGL}^2} \right\}, n \right];$$

 ${\tt ln[25]:= mel2 = SumToMellin[sum2, C, x, ToGLbBasis \rightarrow False]}$ 

$$\begin{array}{l} \text{Out}[25]= \end{array} \left\{ \frac{2\sqrt{2} \; \texttt{Mellin}\left((-4)^n x^n - 1, \frac{\sqrt{x}(\texttt{Hwb}[\{\texttt{fw6},\texttt{fw1},\texttt{fw1}\},\texttt{x}] - \texttt{22} \; \texttt{Hwb}[\{\texttt{fw6}\},\texttt{x}])}{\sqrt{1 - \frac{x}{2}}(4\texttt{x} + 1)}\right)}{\pi} \\ + \frac{5 \; \texttt{z3} \; \texttt{Mellin}\left((-8)^n x^n - 1, \frac{\sqrt{x}}{\sqrt{1 - x}\left(\texttt{x} + \frac{1}{8}\right)}\right)}{8\pi}, \{\} \end{array} \right\} \end{array}$$

where

$$f_{w_1}(x) = \frac{1}{\sqrt{x(1-x)}}, \quad f_{w_6}(x) = \frac{1}{\sqrt{1-x}\sqrt{2-x}}$$

ln[26]:= asymp2 = AsymptoticsSum[sum2, n, x, 5]

$$5\left(-\frac{13\sqrt{\pi}(-8)^n}{818^{3/2}}-\frac{13\sqrt{\pi}(-1)^n2^{3n-4}}{2438^{5/2}}+\frac{2195\sqrt{\pi}(-1)^n2^{3n-7}}{2187n^{7/2}}+\frac{806953\sqrt{\pi}(-1)^n8^{n-4}}{196838^{9/2}}+\frac{\sqrt{\pi}(-1)^n8^{n+1}}{9\sqrt{n}}\right)z3^{3/2}$$

 $8\pi$ 

ln[28]:= asymp2 = AsymptoticsSum[sum2, n, x, 5]

# Conclusion

- Both Mellin inversion and asymptotics computation presented [Iterated Binomial Sums and their Associated Iterated Integrals by J. Ablinger, J. Blümlein, C.G. Raab and C. Schneider] implemented in the package
- We have extended the inversion method to make it work with some new classes of binomial nested sums (e.g. involving some classes of rational functions)
- Fully symbolic representation of constants
- Asymptotic expansion of sums with several possible schemes

### Work in progress

- Explicit computation/simplification of constants is highly non-trivial, structure of binomial sums needs to be explored further (building a basis of binomial sums, unicity of root alphabet/relation between letters,...)
- Some classes of convolution involve difficult integrals that need to be tackled properly

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## Thank you for listening!

J. Ablinger, J. Blümlein, and C.Schneider. "Analytic and algorithmic aspects of generalized harmonic sums and polylogarithms". In: *Journal of Mathematical Physics* 54.8 (Aug. 2013), p. 082301. DOI: 10.1063/1.4811117. URL: https://doi.org/10.1063%2F1.4811117.

- J. Ablinger et al. "Iterated binomial sums and their associated iterated integrals". In: Journal of Mathematical Physics 55.11 (Nov. 2014), p. 112301. DOI: 10.1063/1.4900836. URL: https://doi.org/10.1063%2F1.4900836.
- J. Ablinger et al. "The O(as3 TF2) contributions to the gluonic operator matrix element". In: *Nuclear Physics B* 885 (Aug. 2014), pp. 280–317. DOI: 10.1016/j.nuclphysb.2014.05.028. URL: https://doi.org/10.1016%2Fj.nuclphysb.2014.05.028.
- Jakob Ablinger, Johannes Blumlein, and Carsten Schneider. "Harmonic Sums and Polylogarithms Generated by Cyclotomic Polynomials". In: J. Math. Phys. 52 (2011), p. 102301. DOI: 10.1063/1.3629472. arXiv: 1105.6063 [math-ph].

- Jakob Ablinger et al. "Calculating massive 3-loop graphs for operator matrix elements by the method of hyperlogarithms". In: *Nuclear Physics B* 885 (Aug. 2014), pp. 409–447. DOI: 10.1016/j.nuclphysb.2014.04.007. URL: https://doi.org/10.1016%2Fj.nuclphysb.2014.04.007.
- Johannes Blumlein and Stefan Kurth. "Harmonic sums and Mellin transforms up to two loop order". In: *Phys. Rev. D* 60 (1999), p. 014018. DOI: 10.1103/PhysRevD.60.014018. arXiv: hep-ph/9810241.
- Christian Krattenthaler and Carsten Schneider. Evaluation of binomial double sums involving absolute values. 2020. arXiv: 1607.05314 [math.CO].
- N. Nielsen. Handbuch der Theorie der Gammafunktion. B.G.Teubner, Leipzig, 1906.
- E. Remiddi and J. A. M. Vermaseren. "Harmonic polylogarithms". In: *Int. J. Mod. Phys. A* 15 (2000), pp. 725–754. DOI: 10.1142/S0217751X00000367. arXiv: hep-ph/9905237.
  - J. A. M. Vermaseren. "Harmonic sums, Mellin transforms and integrals". In: Int. J. Mod. Phys. A 14 (1999), pp. 2037–2076. DOI: 10.1142/S0217751X99001032. arXiv: hep-ph/9806280.

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