## 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:

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

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

- Example 2 (physics): Particle physics computations are often done in Mellin space, and for example in the paper [The $\mathcal{O}\left(\alpha_{s}^{3} T_{F}^{2}\right)$ 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{2 n}{n}\left(\sqrt{\sum_{i=1}^{n} \frac{4^{i}}{i^{2}\binom{2 i}{i}} S_{1}(i-1)}-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:

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

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:

$$
B S_{\left\{a_{1}, \ldots, a_{k}\right\}}(n):=\sum_{i_{1}=1}^{n} a_{1}\left(i_{1}\right) \sum_{i_{2}=1}^{i_{1}} a_{2}\left(i_{2}\right) \cdots \sum_{i_{k}=1}^{i_{k-1}} a_{k}\left(i_{k}\right)
$$

with

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

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

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

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- More generic summands can also be considered, such as:

$$
\frac{c^{n}}{(2 n+1)\binom{2 n}{n}} \text { or } \frac{p(i)}{q(i)}\binom{2 i}{i}, p, q \in \mathbb{C}[X], \operatorname{deg} p \leq \operatorname{deg} q, \operatorname{roots}(q) \subset \mathbb{C} \backslash \mathbb{R}_{+}
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& \text {Example : } \quad \sum_{i=1}^{n} \frac{1+i}{i^{2}+5 i+6} \sum_{j=1}^{i} \frac{(-2)^{j}}{(2 j+1)\binom{2 j}{j}} \sum_{k=1}^{j} \frac{3^{k}}{k^{2}}
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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 $(c \in \mathbb{C})$ :

$$
\begin{equation*}
\sum_{i=1}^{n} c^{i} M[f(x)](i)=c^{n} M\left[\frac{x}{x-\frac{1}{c}} f(x)\right](n)-M\left[\frac{x}{x-\frac{1}{c}} f(x)\right] \tag{1}
\end{equation*}
$$

- Convolution:

$$
\begin{aligned}
f(x) * g(x):= & \int_{0}^{1} \mathrm{~d} x_{1} \int_{0}^{1} \mathrm{~d} x_{2} \delta\left(x-x_{1} x_{2}\right) f\left(x_{1}\right) g\left(x_{2}\right)=\int_{x}^{1} \mathrm{~d} y \frac{f(y)}{y} g\left(\frac{x}{y}\right) \\
& M[f(x) * g(x)](n)=M[f(x)](n) \cdot M[g(x)](n)
\end{aligned}
$$

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- 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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Cons: If the DE cannot be solved (not first-order factorizable or Kovacic method doesn't work), a Mellin representation cannot be obtained

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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 Associated Iterated Integrals by J. Ablinger, J. Blümlein, C.G. Raab and C. Schneider]

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Cons: Different cases have to be identified and implemented individually

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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

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

Defined over a 37 letter alphabet $\left\{f_{0}, \ldots, f_{w_{32}}\right\}$ 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]
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## Example:

$$
\begin{aligned}
\mathrm{H}_{\mathrm{f}_{11}, \mathrm{f}_{2}, \mathrm{f}_{\mathrm{w}}^{8}}
\end{aligned}=\int_{x}^{1} \mathrm{~d} t_{1} f_{w_{11}}\left(t_{1}\right) \int_{t_{1}}^{1} \mathrm{~d} t_{2} f_{2}\left(t_{2}\right) \int_{t_{2}}^{1} \mathrm{~d} t_{3} f_{w_{8}}\left(t_{3}\right) ~(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}}} .
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Example: (linearization by shuffle relations)

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

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:

$$
B S(n)=\sum_{k=1}^{n}\binom{2 i}{i} S_{2}(i)=\sum_{k=1}^{n}\binom{2 i}{i} \sum_{j=1}^{i} \frac{1}{i^{2}}
$$

- 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

$$
\mathrm{H}_{0}^{*}(x):=\int_{x}^{1} \mathrm{~d} t f_{0}(t)=\int_{x}^{1} \mathrm{~d} t \frac{1}{t}=-\log x
$$

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

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

where

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

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$$
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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:

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

So that

$$
\begin{equation*}
\sum_{i=1}^{k}\binom{2 i}{i} S_{2}(i)=\frac{1}{\pi} \sum_{i=1}^{n} 4^{i} M\left[\frac{1}{\sqrt{x(1-x)}}\right](i) \cdot M\left[\frac{\mathrm{H}_{0}^{*}(x)}{x-1}\right](i)+\frac{\zeta_{2}}{\pi} \sum_{i=1}^{k} 4^{i} M\left[\frac{1}{\sqrt{x(1-x)}}\right] \tag{i}
\end{equation*}
$$

- 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{(4 x)^{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:

$$
\begin{equation*}
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] \tag{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:

$$
\begin{equation*}
M\left[\frac{\mathrm{H}_{\mathrm{b}^{\mathrm{w}} \mathrm{w}_{1}}^{*}(x)}{\sqrt{x(x-1)}}\right](i)=-M\left[\frac{\mathrm{H}_{\mathrm{w}_{1}}^{*}(x)^{2}}{2 \sqrt{x(1-x)}}\right] \tag{i}
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\end{equation*}
$$

- Finally, using once again the summation formula we get:

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

and resumming everything, we get:

$$
\sum_{i=1}^{n}\binom{2 i}{i} S_{2}(i)=-\frac{1}{\pi} \int_{0}^{1} \mathrm{~d} x \frac{(4 x)^{n}-1}{x-\frac{1}{4}} \sqrt{\frac{x}{1-x}}\left(\frac{\mathrm{H}_{\mathrm{w}_{1}}^{*}(x)^{2}}{2}-\zeta_{2}\right)
$$

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

$$
\begin{equation*}
\tilde{M}_{a}[f(x)](n):=\int_{0}^{1} \mathrm{~d} x \frac{(a x)^{n}-1}{x-\frac{1}{a}} f(x)=\int_{0}^{1} \mathrm{~d} x\left[(a x)^{n}-1\right] \tilde{f}(x) \tag{2}
\end{equation*}
$$

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 [Iterated 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 $a^{n}$ :

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

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

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 $a^{n}$ :

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

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

- 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:

$$
M\left[\frac{f(x)}{x-\frac{1}{a}}\right](n)=a^{n} \int_{0}^{+\infty} \mathrm{d} z e^{-z n} \underbrace{\frac{e^{-z}}{e^{-z}-1} f\left(e^{-z}\right)}_{=: g(z)}
$$

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

$$
g(z) \underset{z \rightarrow 0}{=} \sum_{\alpha \leq p} g_{\alpha} z^{\alpha}+\mathcal{O}\left(z^{\alpha+1}\right), \quad \alpha \in \frac{1}{2} \mathbb{Z} \geq-1, g_{\alpha} \in \mathbb{R}
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$$

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

$$
\begin{aligned}
\tilde{M}_{a}[f(x)](n) & =a_{n \rightarrow+\infty}^{n} \sum_{\alpha \leq p} \int_{0}^{+\infty} \mathrm{d} z e^{-z n} g_{\alpha} z^{\alpha} \\
& =a^{n} \sum_{\alpha \leq p} \frac{h_{\alpha}}{n^{\alpha}}, \quad h_{\alpha} \in \mathbb{R}
\end{aligned}
$$

First we preload Sigma and HarmonicSums:
$\ln [1]:=\ll$ Sigma.m;
Sigma - A summation package by Carsten Schneider - (c) RISC
$\ln [2]:=\ll$ HarmonicSums.m;
HarmonicSums by Jakob Ablinger - (c) RISC
And then our package:
$\ln [3]:=\ll$ RICA.m;
Rule Induced Convolutions for Asymptotics (RICA) package by Nikolai Fadeev © RISC-JKU

First we preload Sigma and HarmonicSums:
$\ln [6]:=\ll$ Sigma.m;
Sigma - A summation package by Carsten Schneider - (c) RISC
$\ln [7]:=\ll$ HarmonicSums.m;
HarmonicSums by Jakob Ablinger - (c) RISC
And then our package:
$\ln [8]:=\ll$ 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:

$$
\operatorname{In}[9]:=\operatorname{sum} 1=\mathbf{G S}\left[\left\{\operatorname{Binomial}[\mathbf{2} \operatorname{VarGL}, \operatorname{VarGL}], \frac{\mathbf{1}}{\operatorname{VarGL}}{ }^{2}\right\}, \mathbf{n}\right] ;
$$

First we preload Sigma and HarmonicSums:
$\ln [11]:=\ll$ Sigma.m;
Sigma - A summation package by Carsten Schneider - (c) RISC
$\ln [12]:=\ll$ HarmonicSums.m;
HarmonicSums by Jakob Ablinger - (c) RISC
And then our package:
$\ln [13]:=\ll$ 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: $\ln [14]:=\operatorname{sum} 1=\mathbf{G S}\left[\left\{\right.\right.$ Binomial $\left.[\mathbf{2} \operatorname{VarGL}, \operatorname{VarGL}], \frac{1}{\operatorname{VarGL}}\right\}$
We can now compute the Mellin representation:
$\ln [15]:=$ mel1 $=$ SumToMellin[sum1, C, x]
$\operatorname{Out}[15]=\left\{-\frac{2 \operatorname{Mellin}\left(4^{n} x^{n}-1, \frac{\sqrt{x}\left(\operatorname{Hwb}[\{f \mathrm{fw} 1\}, x]^{2}-2 z 2\right)}{\sqrt{1-\mathrm{x}}(4 \mathrm{x}-1)}\right)}{\pi},\{ \}\right\}$

We can now compute the asymptotics, either from the Mellin representation... $\ln [16]$ ]: $\mathbf{a s y m p} 1=$ AsymptoticsMellint[mel1[[1]], $\mathrm{x}, \mathrm{n}, 4]$

Out[16]=

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

We can now compute the asymptotics, either from the Mellin representation... $\operatorname{In}[17]:=\mathbf{a s y m p} 1=$ AsymptoticsMellint[mel1[[1]], $\mathbf{x}, \mathbf{n}, 4]$

Out[17]=

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

...or directly from the sum representation:
$\ln [18]:=\boldsymbol{a s y m p} 1 \mathbf{P}=$ AsymptoticsSum[sum1, n, x, 3]
$\begin{aligned} \text { Out }[18]=- & \frac{2}{\pi}\left(-\frac{(\pi-12)(12+\pi) \sqrt{\pi} 2^{2 n-3}}{27 \mathrm{n}^{3 / 2}}-\frac{\left(288+59 \pi^{2}\right) \sqrt{\pi} 2^{2 \mathrm{n}-7}}{27 \mathrm{n}^{5 / 2}}-\frac{97\left(25 \pi^{2}-432\right) \sqrt{\pi} 2^{2 \mathrm{n}-10}}{81 \mathrm{n}^{7 / 2}}\right. \\ & \left.-\frac{17\left(33929 \pi^{2}-440640\right) \sqrt{\pi} 2^{2 \mathrm{n}-15}}{243 \mathrm{n}^{9 / 2}}-\frac{\pi^{5 / 2} 2^{2 \mathrm{n}}}{9 \sqrt{\mathrm{n}}}\right)\end{aligned}$

We can now compute the asymptotics, either from the Mellin representation... $\operatorname{In}[19]:=\mathbf{a s y m p} 1=$ AsymptoticsMellint[mel1[[1]], $\mathbf{x}, \mathbf{n}, 4]$

Out[19]=

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

$\ln [20]:=$ DiscretePlot $\left[\frac{\mid \text { sum } 1-\text { asymp } 1 \mid}{\mid \text { sum } 1 \mid},\{\mathbf{n}, \mathbf{1}, \mathbf{5 0}\}\right]$
Out[20]=


Here's another example:
$\ln [21]:=\operatorname{sum} 2=\mathbf{G S}\left[\left\{(\mathbf{- 2})^{\text {VarGL }}\right.\right.$ Binomial $\left.\left.[\mathbf{2 V a r G L}, \operatorname{VarGL}], \frac{\left(\frac{1}{2}\right)^{\operatorname{VarGL}}}{\operatorname{VarGL}}, \frac{\mathbf{1}}{\operatorname{VarGL}}\right\}, \mathrm{n}\right]$;

Here's another example:
$\ln [22]:=\operatorname{sum} 2=\mathbf{G S}\left[\left\{(\mathbf{- 2})^{\operatorname{VarGL}}\right.\right.$ Binomial $\left.\left.[\mathbf{2 V a r G L}, \operatorname{VarGL}], \frac{\left(\frac{1}{2}\right)^{\operatorname{VarGL}}}{\operatorname{VarGL}}, \frac{\mathbf{1}}{\operatorname{VarGL}}\right\}, \mathrm{n}\right]$; $\ln [23]:=$ ToHarmonicSumsSum[sum2]
Out [23]= $\sum_{\tau_{1}=1}^{\mathrm{n}}(-2)^{\tau_{1} \text { Binomial }\left[2 \tau_{1}, \tau_{1}\right]}\left(\sum_{\tau_{2}=1}^{\tau_{1}} \frac{2^{-\tau_{2}}\left(\sum_{\tau_{3}=1}^{\tau_{2}} \frac{1}{\tau_{3}^{2}}\right)}{\tau_{2}}\right)$

Here's another example:
$\ln [24]:=\operatorname{sum} 2=\mathbf{G S}\left[\left\{(\mathbf{- 2})^{\text {VarGL }}\right.\right.$ Binomial $\left.\left.[2 \operatorname{VarGL}, \operatorname{VarGL}], \frac{\left(\frac{1}{2}\right)^{\operatorname{VarGL}}}{\operatorname{VarGL}}, \frac{\mathbf{1}}{\operatorname{VarGL}}\right\}, \mathbf{n}\right]$;
$\ln [25]:=$ mel2 $=$ SumToMellin[sum2, C, $\mathbf{x}$, ToGLbBasis $\rightarrow$ False]
$\operatorname{Out}[25]=\left\{\begin{array}{l}2 \sqrt{2} \operatorname{Mellin}\left((-4)^{n} x^{n}-1, \frac{\sqrt{x}(H w b[\{f w 6, f w 1, f w 1\}, x]-z 2 \operatorname{Hwb}[\{f w 6\}, x])}{\sqrt{1-\frac{x}{2}}(4 x+1)}\right) \\ \pi\end{array}\right.$

$$
\left.+\frac{5 \text { z3 Mellin }\left((-8)^{n} x^{n}-1, \frac{\sqrt{x}}{\sqrt{1-x}\left(x+\frac{1}{8}\right)}\right)}{8 \pi},\{ \}\right\}
$$

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]

Out[26]=

$$
\frac{5\left(-\frac{13 \sqrt{\pi}(-8)^{\mathrm{n}}}{81 \mathrm{n}^{3 / 2}}-\frac{13 \sqrt{\pi}(-1)^{\mathrm{n}} 2^{3 \mathrm{n}-4}}{243 \mathrm{n}^{5 / 2}}+\frac{2195 \sqrt{\pi}(-1)^{\mathrm{n}} 2^{3 \mathrm{n}-7}}{2187 \mathrm{n}^{7 / 2}}+\frac{806953 \sqrt{\pi}(-1)^{\mathrm{n}} 8^{\mathrm{n}-4}}{19683 \mathrm{n}^{9 / 2}}+\frac{\sqrt{\pi}(-1)^{\mathrm{n}} 8^{\mathrm{n}+1}}{9 \sqrt{\mathrm{n}}}\right) \mathrm{z} 3}{8 \pi}
$$

$\ln [28]:=$ asymp2 $=$ AsymptoticsSum[sum2, n, $\mathbf{x}, \mathbf{5}]$
Out[28]=

$$
\frac{5\left(-\frac{13 \sqrt{\pi}(-8)^{\mathrm{n}}}{81 \mathrm{n}^{3 / 2}}-\frac{13 \sqrt{\pi}(-1)^{\mathrm{n}} 2^{3 \mathrm{n}-4}}{243 \mathrm{n}^{5 / 2}}+\frac{2195 \sqrt{\pi}(-1)^{\mathrm{n}} 2^{3 \mathrm{n}-7}}{2187 \mathrm{n}^{7 / 2}}+\frac{806953 \sqrt{\pi}(-1)^{\mathrm{n}} 8^{\mathrm{n}-4}}{19683 \mathrm{n}^{9 / 2}}+\frac{\sqrt{\pi}(-1)^{\mathrm{n}} 8^{\mathrm{n}+1}}{9 \sqrt{\mathrm{n}}}\right) \mathrm{z} 3}{8 \pi}
$$

$\operatorname{In}[29]:=$ DiscretePlot $\left[\frac{\mid \text { sum } 2-\text { asymp2| }}{\mid \text { sum } 2 \mid},\{\mathbf{n}, \mathbf{1}, \mathbf{5 0}\}\right]$
Out[29]=


## 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.
T. 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.
國 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.
T. 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].
目 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.
E. 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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