

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

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July 25, 2023

Supported by the Austrian Science Foundation (FWF) grant P33530.



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:

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

If we want the asymptotic expansion at $m \rightarrow +\infty$ for fixed n , 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 $\mathcal{O}(\alpha_s^3 T_F^2)$ contributions to the gluonic operator matrix element* by J.Ablinger, J. Blümlein, C. Schneider et al.], sums of the following form pop up:

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

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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:

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

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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 :

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

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

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

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

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

► Definition:

$$M[f(x)](n) := \int_0^1 dx x^n f(x)$$

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

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

► Convolution:

$$f(x) * g(x) := \int_0^1 dx_1 \int_0^1 dx_2 \delta(x - x_1 x_2) f(x_1) g(x_2) = \int_x^1 dy \frac{f(y)}{y} g\left(\frac{x}{y}\right)$$

$$M[f(x) * g(x)](n) = M[f(x)](n) \cdot M[g(x)](n)$$

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

Note: These Mellin representations will involve general polylogarithms

$$H_{\emptyset}^*(x) := 1, \quad H_{\mathbf{b}(t), \vec{c}(t)}^*(x) = H_{\mathbf{b}, \vec{c}}^*(x) := \int_x^1 dt b(t) H_{\vec{c}}^*(t)$$

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

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Example:

$$\begin{aligned} H_{f_{w_{11}}, f_2, f_{w_8}}^* &= \int_x^1 dt_1 f_{w_{11}}(t_1) \int_{t_1}^1 dt_2 f_2(t_2) \int_{t_2}^1 dt_3 f_{w_8}(t_3) \\ &= \int_x^1 dt_1 \frac{1}{t_1 \sqrt{1-t_1} \sqrt{2-t_1}} \int_{t_1}^1 dt_2 \frac{1}{2-t_2} \int_{t_2}^1 dt_3 \frac{1}{t_3 \sqrt{t_3 - \frac{1}{4}}} \end{aligned}$$

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Example: (linearization by shuffle relations)

$$H_{f_1}^*(x) H_{f_0, f_{-1}}^*(x) = H_{f_1, f_0, f_{-1}}^*(x) + H_{f_0, f_{-1}, f_1}^*(x) + H_{f_0, f_1, f_{-1}}^*(x)$$

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:

$$\frac{1}{i^2} = M \left[\frac{1}{x} \right] (i) \cdot M \left[\frac{1}{x} \right] (i) = M \left[\frac{1}{x} * \frac{1}{x} \right] (i) = M \left[\frac{H_0^*(x)}{x} \right] (i)$$

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:

$$S_2(i) = \sum_{k=1}^i M \left[\frac{H_0^*(x)}{x} \right] (i) = \underbrace{\int_0^1 dx x^i \frac{H_0^*(x)}{x-1}}_{M \left[\frac{x}{x-1} \frac{H_0^*(x)}{x} \right] (i)} - \underbrace{\int_0^1 dx \frac{H_0^*(x)}{x-1}}_{M \left[\frac{x}{x-1} \frac{H_0^*(x)}{x} \right] (0)} = \int_0^1 dx x^i \frac{H_0^*(x)}{x-1} + \zeta_2$$

where

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- ▶ Now that the innermost sum has an 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

$$\sum_{i=1}^k \binom{2i}{i} S_2(i) = \frac{1}{\pi} \sum_{i=1}^n 4^i M \left[\frac{1}{\sqrt{x(1-x)}} \right] (i) \cdot M \left[\frac{H_0^*(x)}{x-1} \right] (i) + \frac{\zeta_2}{\pi} \sum_{i=1}^k 4^i M \left[\frac{1}{\sqrt{x(1-x)}} \right] (i)$$

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

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

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

$$M \left[\frac{1}{\sqrt{x(1-x)}} \right] (i) \cdot M \left[\frac{H_0^*(x)}{x-1} \right] (i) = M \left[\int_x^1 dy \frac{H_0^*(y)}{(y-1)\sqrt{y-x}} \right] (i)$$

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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:

$$\int_x^1 dy \frac{H_0^*(y)}{(y-1)\sqrt{y-x}} = \frac{H_{b,w_1}^*(x)}{\sqrt{x-1}}, f_b(x) = \frac{1}{\sqrt{x(x-1)}}, f_{w_1}(x) = \frac{1}{\sqrt{x(1-x)}}$$

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

$$M \left[\frac{H_{b,w_1}^*(x)}{\sqrt{x(x-1)}} \right] (i) = -M \left[\frac{H_{w_1}^*(x)^2}{2\sqrt{x(1-x)}} \right] (i)$$

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

$$\sum_{i=1}^n 4^i M \left[\frac{H_{w_1}^*(x)^2}{2\sqrt{x(1-x)}} \right] (i) = \int_0^1 dx \frac{(4x)^n - 1}{x - \frac{1}{4}} \sqrt{\frac{x}{1-x}} \frac{H_{w_1}^*(x)^2}{2}$$

and resumming everything, we get:

$$\sum_{i=1}^n \binom{2i}{i} S_2(i) = -\frac{1}{\pi} \int_0^1 dx \frac{(4x)^n - 1}{x - \frac{1}{4}} \sqrt{\frac{x}{1-x}} \left(\frac{H_{w_1}^*(x)^2}{2} - \zeta_2 \right)$$

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

$$\tilde{M}_a[f(x)](n) := \int_0^1 dx \frac{(ax)^n - 1}{x - \frac{1}{a}} f(x) = \int_0^1 dx [(ax)^n - 1] \tilde{f}(x) \quad (2)$$

where

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

- ▶ There exist several methods 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 :

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

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

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- In $M \left[\frac{f(x)}{x - \frac{1}{a}} \right] (n)$, we make the following change of variables:

$$x = e^{-z}, \quad dx = -e^{-z} dz$$

and end up with:

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

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

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

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

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

- ▶ 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:

$$\begin{aligned} \tilde{M}_a[f(x)](n) &\underset{n \rightarrow +\infty}{=} a^n \sum_{\alpha \leq p} \int_0^{+\infty} dz e^{-zn} g_{\alpha} z^{\alpha} \\ &= a^n \sum_{\alpha \leq p} \frac{h_{\alpha}}{n^{\alpha}}, \quad h_{\alpha} \in \mathbb{R} \end{aligned}$$

First we preload Sigma and HarmonicSums:

```
In[1]:= << Sigma.m;
```

Sigma - A summation package by Carsten Schneider – © RISC

```
In[2]:= << HarmonicSums.m;
```

HarmonicSums by Jakob Ablinger – © RISC

And then our package:

```
In[3]:= << RICA.m;
```

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

First we preload Sigma and HarmonicSums:

```
In[6]:= << Sigma.m;
```

Sigma - A summation package by Carsten Schneider – © RISC

```
In[7]:= << HarmonicSums.m;
```

HarmonicSums by Jakob Ablinger – © RISC

And then our package:

```
In[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]:= sum1 = GS [ { Binomial[2 VarGL, VarGL],  $\frac{1}{\text{VarGL}^2}$  }, n ] ;
```

First we preload Sigma and HarmonicSums:

```
In[11]:= << Sigma.m;
```

Sigma - A summation package by Carsten Schneider – © RISC

```
In[12]:= << HarmonicSums.m;
```

HarmonicSums by Jakob Ablinger – © RISC

And then our package:

```
In[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]:= sum1 = GS [ { Binomial[2 VarGL, VarGL],  $\frac{1}{\text{VarGL}^2}$  }, n ] ;
```

We can now compute the Mellin representation:

```
In[15]:= mel1 = SumToMellin[sum1, C, x]
```

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

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

```
In[16]:= asympt1 = AsymptoticsMellint[mel1[[1]], x, n, 4]
```

```
Out[16]=
```

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

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

```
In[17]:= asympt1 = AsymptoticsMellin[mel1[[1]], x, n, 4]
```

```
Out[17]=
```

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

...or directly from the sum representation:

```
In[18]:= asympt1P = AsymptoticsSum[sum1, n, x, 3]
```

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

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

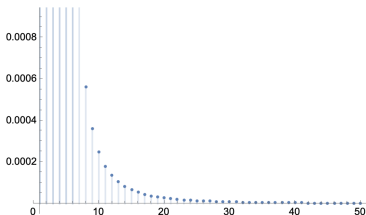
```
In[19]:= asymp1 = AsymptoticsMellint[mel1[[1]], x, n, 4]
```

```
Out[19]=
```

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

```
In[20]:= DiscretePlot [  $\frac{|\text{sum1} - \text{asymp1}|}{|\text{sum1}|}$ , {n, 1, 50} ]
```

```
Out[20]=
```



Here's another example:

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

Here's another example:

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

`In[23]:= ToHarmonicSumsSum[sum2]`

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

Here's another example:

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

$$\text{In[25]:= mel2} = \text{SumToMellin}[\text{sum2}, \mathbf{C}, \mathbf{x}, \text{ToGLbBasis} \rightarrow \text{False}]$$

$$\text{Out[25]=} \left\{ \frac{2\sqrt{2} \text{ Mellin} \left((-4)^n x^n - 1, \frac{\sqrt{x}(\text{Hwb}[\{\text{fw6}, \text{fw1}, \text{fw1}\}, x] - z2 \text{Hwb}[\{\text{fw6}\}, x])}{\sqrt{1 - \frac{x}{2}(4x+1)}} \right)}{\pi} \right. \\ \left. + \frac{5 z3 \text{ Mellin} \left((-8)^n x^n - 1, \frac{\sqrt{x}}{\sqrt{1-x} \left(x + \frac{1}{8}\right)} \right)}{8\pi}, \{\} \right\}$$

where

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

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

Out[26]=

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

8π

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

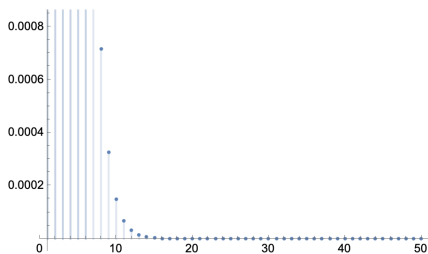
Out[28]=

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

8π

In[29]:= **DiscretePlot** $\left[\frac{|\text{sum2} - \text{asymp2}|}{|\text{sum2}|}, \{\mathbf{n}, 1, 50\} \right]$

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





Conclusion







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Thank you for listening!

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