Binomial Sums in the package HarmonicSums

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Der Wissenschaftsfonds.

Binomial Sums

J.A., Blümlein, Borwein, Broadhurst, Davydychev, Fleischer, Jegerlehner, Kalmykov, Kamnitzer, Kotikov, Lehmer, Lisoněk, Ogreid, Osland, Raab, Schneider, Sun, Weinzierl, Veretin, Ward, Yost, Zucker,. . .

For $a_i, c_i \in \mathbb{N}$, $b_i \in \mathbb{N}_0$, $x_i \in \mathbb{R}^*$, $d_i \in \mathbb{Z}$ and $n \in \mathbb{N}$ we define

$$\mathsf{S}_{(a_1,b_1,c_1,d_1,x_1),\ldots,(a_k,b_k,c_k,d_k,x_k)}(n) = \sum_{i=1}^{n} \frac{{x_1}^i}{(a_1 i + b_1)^{c_1}} \binom{2i}{i}^{d_1} \mathsf{S}_{(a_2,b_2,c_2,d_2,x_2),\ldots,(a_k,b_k,c_k,d_k,x_k)}(n)$$

and $\mathsf{S}(n) = 1$.

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and $\mathsf{S}\,(n) = 1$.

$$\mathsf{S}_{(1,0,3,0,1),(1,0,2,0,-1)}(n) \quad = \quad \sum_{i=1}^{n} \frac{\sum_{j=1}^{i} \frac{(-1)^j}{j^2}}{i^3}$$

harmonic sums: Vermaseren 98; Blümlein, Kurth 98

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- quasi shuffle algebra
- shift: $m_i = (a_i, b_i, c_i, d_i, x_i)$

$$\mathsf{S}_{m_1,m_2,\ldots,m_k}(n+1) = \mathsf{S}_{m_1,\ldots,m_k}(n) + \frac{{x_1}^{n+1}}{(a_1(n+1)+b_1)^{c_1}} \binom{2(n+1)}{n+1}^{d_1} \mathsf{S}_{m_2,\ldots,m_k}(n+1)$$

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we can express that letter:
$$\sum_{i_1=1}^{n} p(i_1) \sum_{i_2=1}^{i_1} f(i_2) \sum_{i_3=1}^{i_2} q(i_3) = \frac{1}{c}\left(-\sum_{i=1}^{k} c_i \sum_{i_1=1}^{n} p(i_1) \sum_{i_2=1}^{i_1} f_i(i_2) \sum_{i_3=1}^{i_2} q(i_3) + \sum_{i_1=1}^{n} p(i_1) g(i_1+1) \sum_{i_2=1}^{i_1+1} q(i_2) - \sum_{i_1=1}^{n} p(i_1) \sum_{i_2=1}^{i_1+1} g(i_2) q(i_2)\right)$$

We consider the following sums:

$$\sum_{i=1}^{n} \frac{1}{i\binom{2i}{i}}, \sum_{i=1}^{n} \frac{1}{(1+i)\binom{2i}{i}}, \sum_{i=1}^{n} \frac{1}{(2+i)\binom{2i}{i}}$$

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With a variant of Gosper's algorithm we can check that there are no c_i and $g(n)$ such that

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And hence we get

$$\begin{aligned}\sum_{i=1}^{n} \frac{1}{(2+i)\binom{2i}{i}} &= -2\sum_{i=1}^{n} \frac{1}{i\binom{2i}{i}} + 6\sum_{i=1}^{n} \frac{1}{(1+i)\binom{2i}{i}} \\ &\quad + \frac{1}{(2+n)\binom{2n}{n}} - \frac{1}{2+n} - \frac{n}{2(2+n)}\end{aligned}$$

Iterated Integrals over Root-valued Alphabets

compare J.A., Blümlein, Raab, Schneider 2014

We introduce a general class of iterated integrals which we define recursively by

$$\mathsf{G}\left(f_1(\tau), f_2(\tau), \cdots, f_k(\tau), x\right) = \int_0^x f_1(\tau_1) \mathsf{G}\left(f_2(\tau), \cdots, f_k(\tau), \tau_1\right) d\tau_1$$

with the special cases

$$\mathsf{G}\left(x\right) = 1$$

and

$$\mathsf{G}\Bigg(\underbrace{\frac{1}{\tau}, \frac{1}{\tau}, \ldots, \frac{1}{\tau}}_{k \text{ times}}, x\Bigg) = \frac{1}{k!} \log(x)^k.$$

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Concidering the letters

$$\frac{1}{\tau}, \frac{1}{1+\tau}, \frac{1}{1-\tau}$$

leads to harmonic polylogarithms. Remiddi, Vermaseren 2000

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- differentiation:

$$\frac{d}{dx}\mathsf{G}\left(f_1(\tau), f_2(\tau), \cdots, f_k(\tau), x\right) = f_1(x)\mathsf{G}\left(f_2(\tau), \cdots, f_k(\tau), x\right)$$

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$$\int_0^x p(y) \int_0^y f(z) \int_0^z q(w)dwdzdy =$$
$$\frac{1}{c}\left(-\sum_{i=1}^{k} c_i \int_0^x p(y) \int_0^y f_i(z) \int_0^z q(w)dwdzdy \right.$$
$$\left. + \int_0^x p(y)g(y) \int_0^y q(w)dwdy - \int_0^x p(y) \int_0^y g(z)q(z)dzdy \right)$$

$$\mathsf{G}\left((1+\tau)^{\frac{3}{2}}, \frac{1}{2+\tau}, \frac{\sqrt{1+\tau}}{2+\tau}, x\right) =$$

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$$\frac{2}{5}(x+1)^{\frac{5}{2}}\mathsf{G}\left(\frac{1}{2+\tau_1}, \frac{\sqrt{1+\tau}}{2+\tau}, x\right) - \frac{2}{5}\mathsf{G}\left(\frac{\sqrt{1+\tau}}{2+\tau}, \frac{\sqrt{1+\tau}}{2+\tau}, x\right)$$
$$-\frac{4}{75}(3x-2)(x+1)^{\frac{3}{2}}\mathsf{G}\left(\frac{\sqrt{1+\tau}}{2+\tau}, x\right) - \frac{32}{75}\mathsf{G}\left(\frac{1}{2+\tau}, x\right)$$
$$+\frac{4}{75}x\left(x^2-x+3\right)$$

D-finite and P-finite

For details see e.g., The Concrete Tetrahedron (Kauers, Paule).

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- A function $f = f(x)$ is called *D-finite* if there exist $p_d(x), p_{d-1}(x), \ldots, p_0(x) \in \mathbb{K}[x]$ (not all $p_i = 0$) such that

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- A sequence $(f_n)_{n\geq 0} \in \mathbb{K}^{\mathbb{N}}$ is called *P-finite* if there exist $p_d(n), p_{d-1}(n), \ldots, p_0(n) \in \mathbb{K}[n]$ (not all $p_i = 0$) such that

$$p_d(n)f_{n+d} + \cdots + p_1(n)f_{n+1} + p_0(n)f_n = 0.$$

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- We get a linear recurrence equation with polynomial coefficients, satisfied by $(f_n)_{n\geq 0}$.

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Hence

$$(n+1)^3 f_{n+1} - (n+2)(n+1)f_{n+2} - (n+2)(n+3)(n+1)f_{n+3} = 0$$

holds for $(f_n)_{n>0}$.

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Note: This is implemented in `HarmonicSums`.

The reverse direction can be performed as well. For example given

$$f(x) = \sum_{i=1}^{\infty} \frac{x^i \binom{2i}{i}}{i^2}$$

we find:

$$\begin{aligned} f(x) &= \frac{1}{32}\left(16x - 20x^2 + 8x^3 - x^4\right) + \frac{x-2}{8}\sqrt{(4-x)x}\,\mathsf{G}\left(\sqrt{4-\tau}\sqrt{\tau}, x\right) \\ &\quad + \frac{1}{8}\mathsf{G}\left(\sqrt{4-\tau}\sqrt{\tau}, x\right)^2 \end{aligned}$$

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This together with integral substitutions can be used to find and prove identities of the form (see J.A. 2016)

$$\begin{aligned} \sum_{i=1}^{\infty} \frac{\sum_{j=1}^{i} \frac{1}{j^2}}{(1+2i)\binom{2i}{i}} &= \frac{\pi^3}{81\sqrt{3}} \\ \sum_{i=1}^{\infty} \frac{\sum_{j=1}^{i} \frac{1}{j^3}}{i^2\binom{2i}{i}} &= \frac{\zeta_5}{9} + \frac{\pi^2\zeta_3}{27} \\ \sum_{i=1}^{\infty} \frac{4^{-i}\binom{2i}{i}\sum_{j=1}^{i} \frac{4^j \sum_{k=1}^{j}\frac{1}{k}}{j^2\binom{2j}{j}}}{i} &= 7\log(2)\zeta_3. \end{aligned}$$

Mellin transform of D-finite functions

Compare J.A, Blümlein, Raab, Schneider 2014.

Let $f(x)$ be a D-finite function such that

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

exists and let $p_i(x) \in \mathbb{K}[x]$ such that

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Since we have

$$\begin{aligned}\mathbf{M}[x^m f^{(p)}(x)](n) &= \frac{(-1)^p(n+m)!}{(n+m-p)!}\mathbf{M}[f(x)](n+m-p)\\ &\quad+\sum_{i=0}^{p-1}\frac{(-1)^i(n+m)!}{(n+m-i)!}f^{(p-1-i)}(1),\end{aligned}$$

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$$\begin{aligned} \mathbf{M}[x^m f^{(p)}(x)](n) &= \frac{(-1)^p (n+m)!}{(n+m-p)!} \mathbf{M}[f(x)](n+m-p) \\ &\quad + \sum_{i=0}^{p-1} \frac{(-1)^i (n+m)!}{(n+m-i)!} f^{(p-1-i)}(1), \end{aligned}$$

we can conclude:

If the Mellin transform of a D-finite function is defined i.e., the integral $\int_0^1 x^n f(x) dx$ exists, then it is P-finite.

Given a D-finite function $f(x)$.
Find an expression $F(n)$ given as a linear combination of indefinite nested sums such that for all $n \in \mathbb{N}$ (from a certain point on) we have

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1. Compute a D-finite differential equation for $f(x)$.
2. Use the proposition above to compute a P-finite recurrence for $\mathbf{M}[f(x)](n)$.

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3. Compute initial values for the recurrence.
4. Solve the recurrence (using `Sigma`) to get a closed form representation for $\mathbf{M}[f(x)](n)$.

Note: This is implemented in `HarmonicSums`.

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Initial values can be computed easily and solving the recurrence leads to

$$\begin{aligned} \mathbf{M}[f(x)](n) \quad &= \quad (-1)^n\left(\frac{4^{n+1}}{(2n+1)(2n+3)\binom{2n}{n}} + \frac{\mathsf{G}\left(\frac{\sqrt{1-\tau}}{1+\tau}, 1\right) - 2}{n+1}\right) \\ &\quad\;\; - \frac{4(-1)^n \sum_{i=1}^{n} \frac{4^i}{(2i+1)\binom{2i}{i}}}{n+1} + \frac{\mathsf{G}\left(\frac{\sqrt{1-\tau}}{1+\tau}, 1\right)}{n+1}. \end{aligned}$$

Note that this method can be extended to compute regularized Mellin transforms i.e., given a D-finite function $f(x)$ such that

$$\int_0^1 (x^n - 1) f(x) dx$$

exists then we can compute

$$\mathbf{M}[[f(x)]_+](n) := \int_0^1 (x^n - 1) f(x) dx$$

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$$\mathbf{M}\left[\left[\frac{\mathsf{G}\left(\frac{1}{\sqrt{\tau}\sqrt{4-\tau}}, x\right)}{1-x}\right]_+\right](n) = \int_0^1 (x^n - 1)\frac{\mathsf{G}\left(\frac{1}{\sqrt{\tau}\sqrt{4-\tau}}, x\right)}{1-x} dx =$$

$$\frac{1}{6}\left(3\sqrt{3} + 2\pi\right)\left(\sum_{i=1}^{n} \frac{\binom{2i}{i}}{i} - \sum_{i=1}^{n} \frac{1}{i}\right) - \frac{3}{2}\sqrt{3}\sum_{i=1}^{n} \frac{\binom{2i}{i}\sum_{j=1}^{i}\frac{1}{\binom{2j}{j}}}{i}$$

Inverse Mellin transform

Given a P-finite recurrence for **M**$[f(x)](n)$.
Find a differential equation for $f(x)$.

Given a P-finite recurrence for $\mathbf{M}[f(x)](n)$.
Find a differential equation for $f(x)$.

We observe that

$$\begin{aligned} n^p\,\mathbf{M}[f(x)](n+m) \quad &= \quad \mathbf{M}[(-1)^p x^{m+p} f^{(p)}(x)](n) - a(n)\,\mathbf{M}[f(x)](n+m) \\ &\quad - \sum_{i=0}^{p-1} \frac{(-1)^{i+p}(n+m+p)!}{(n+m+p-i)!} f^{(p-1-i)}(1), \end{aligned}$$

where $a(n) \in \mathbb{K}[n]$ with $\deg(a(n)) < p$.

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where $a(n) \in \mathbb{K}[n]$ with $\deg(a(n)) < p$.

We can use this observation to compute the differential equation recursively.

Given the P-finite recurrence for $\mathbf{M}[f(x)](n)$:

$$p_d(n) f_{n+d} + \cdots + p_1(n) f_{n+1} + p_0(n) f_n = 0.$$

Given the P-finite recurrence for $\mathbf{M}[f(x)](n)$:

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Let $k := \max_{0\leq i\leq d}(\deg(p_i(x)))$ and let c be the coefficient of n^k in the recurrence i.e.,

$$c = \sum_{i=0}^{d} c_i f_{n+i}$$

for some $c_i \in \mathbb{K}$.

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for some $c_i \in \mathbb{K}$.
Replace $c_i n^k f_{n+i}$ by

$$c_i n^k f_{n+i} + c_i(-1)^k x^{k+i} f^{(k)}(x) - c_i\,\mathbf{M}[(-1)^k x^{k+i} f^{(k)}(x)](n).$$

Given the P-finite recurrence for $\mathbf{M}[f(x)](n)$:

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This reduces the degree of n.

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This reduces the degree of n.
Apply this strategy until all appearences of $n^p\ f_{n+i}$ are removed, this yields

$$q_l(x)f^{(l)}(x) + \cdots + q_1(x)f'(x) + q_0(x)f(x) + \sum_{j=0}^{k-1} r_j(n)f^{(j)}(1) = 0.$$

where $q_i(n) \in \mathbb{K}[q]$ and $r_j(n) \in \mathbb{K}[n]$.

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We substitute

$$\begin{array}{rcl} nf_{n+2} & \to & nf_{n+2} - x^3 f'(x) + \mathbf{M}[x^3 f'(x)](n) \\ -nf_n & \to & -nf_n + xf'(x) - \mathbf{M}[xf'(x)](n) \end{array}$$

Consider the recurrence

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This yields

$$(-x^3 + x)f' - f_{n+2} - f_{n+1} = 0.$$

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Since

$$\begin{aligned} \mathbf{M}[x^2 f(x)](n) &= f_{n+2} \\ \mathbf{M}[x f(x)](n) &= f_{n+1} \end{aligned}$$

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Note: This is implemented in `HarmonicSums`.

We want to compute the inverse Mellin transform of

$$f_n := (-1)^n \left(\sum_{i=1}^{n} \frac{(-1)^i \sum_{j=1}^{i} \frac{1}{j^2}}{i} - \sum_{i=1}^{\infty} \frac{(-1)^i \sum_{j=1}^{i} \frac{1}{j^2}}{i} \right)$$

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We find that

$$\begin{aligned} 0 \quad = \quad & (n+1)(n+2)^2 f_n - (n+2)\left(n^2+7n+11\right) f_{n+1} \\ & + \left(-n^3-5n^2-6n+1\right) f_{n+2} + (n+3)^3 f_{n+3} \end{aligned}$$

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that has the general solution

$$s(x) = \frac{c_1}{x+1} + \frac{c_2}{x+1} \mathsf{G}\left(\frac{1}{\tau-1}, x\right) + \frac{c_3}{x+1} \mathsf{G}\left(\frac{1}{\tau-1}, \frac{1}{\tau}, x\right),$$

for some constants c_1, c_2, c_3.

In order to determine these constants we compute

$$\begin{aligned}
\int_0^1 x^0 s(x)dx &= c_1 \log(2) + c_2 \frac{\log(2)^2 - \zeta_2}{2} + c_3 \frac{2\zeta_3 - \log(2)\zeta_2}{2} \\
\int_0^1 x^1 s(x)dx &= c_1(1 - \log(2)) + c_2 \frac{-\log(2)^2 + \zeta_2 - 2}{2} + c_3 \frac{\log(2)\zeta_2 - 2\zeta_3 + 2}{2} \\
\int_0^1 x^2 s(x)dx &= c_1 \frac{2\log(2) - 1}{2} + c_2 \frac{2\log(2)^2 - 2\zeta_2 + 1}{4} + c_3 \frac{8\zeta_3 - 4\log(2)\zeta_2 - 3}{8}.
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Since

$$\begin{aligned}
f_0 &= -\sum_{i=1}^{\infty} \frac{(-1)^i \sum_{j=1}^{i} \frac{1}{j^2}}{i} \\
f_1 &= 1 + \sum_{i=1}^{\infty} \frac{(-1)^i \sum_{j=1}^{i} \frac{1}{j^2}}{i} \\
f_2 &= -\frac{3}{8} - \sum_{i=1}^{\infty} \frac{(-1)^i \sum_{j=1}^{i} \frac{1}{j^2}}{i}
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$$\begin{aligned} f_0 &= -\sum_{i=1}^{\infty} \frac{(-1)^i \sum_{j=1}^{i} \frac{1}{j^2}}{i}\\ f_1 &= 1 + \sum_{i=1}^{\infty} \frac{(-1)^i \sum_{j=1}^{i} \frac{1}{j^2}}{i}\\ f_2 &= -\frac{3}{8} - \sum_{i=1}^{\infty} \frac{(-1)^i \sum_{j=1}^{i} \frac{1}{j^2}}{i}\end{aligned}$$

we can deduce that $c_0 = 0, c_1 = 0$ and $c_2 = 1$ and hence

$$f_n = \mathsf{M}\left[\frac{1}{x+1}\mathsf{G}\left(\frac{1}{\tau - 1}, \frac{1}{\tau}, x\right)\right](n).$$

$$\sum_{i=1}^{n}\frac{1}{\binom{2i}{i}i^3} = 4^{-n}\int_0^1 x^n\left(-\frac{\pi^2}{6(-4+x)}+\frac{2\mathsf{G}\left(\frac{1}{\tau},x\right)}{-4+x}-\frac{2\mathsf{G}\left(\frac{\sqrt{1-\tau}}{\tau},x\right)}{-4+x}\right.$$
$$\left.+\frac{\mathsf{G}\left(\frac{1}{\tau},\frac{\sqrt{1-\tau}}{\tau},x\right)}{-4+x}-\frac{2\mathsf{G}\left(\frac{1}{\tau},x\right)\log(2)}{-4+x}+\frac{2\log^2(2)}{-4+x}\right)dx$$
$$+\sum_{i=1}^{\infty}\frac{1}{\binom{2i}{i}i^3}$$

$$\sum_{i=1}^{n}\frac{\binom{2i}{i}\sum_{j=1}^{i}\frac{1}{j^2}}{i} = \int_0^1\left((4\,x)^n-1\right)\left(\frac{4\pi\mathsf{G}\left(\frac{1}{\sqrt{1-\tau}\sqrt{\tau}},x\right)}{-3+12x}\right.$$
$$\left.+\frac{2\mathsf{G}\left(\frac{1}{\sqrt{1-\tau}\sqrt{\tau}},x\right)^2}{1-4x}-\frac{2\mathsf{G}\left(\frac{1}{\sqrt{1-\tau}\sqrt{\tau}},x\right)^3}{3\pi-12\pi x}\right)dx$$

$$\sum_{i=1}^{n} \frac{1}{\binom{2i}{i} i^3} \sim 2^{-2n}\sqrt{n}\sqrt{\pi}\left(\frac{3927237851}{21233664n^8} - \frac{34924547}{884736n^7} + \frac{91999}{9216n^6} - \frac{10537}{3456n^5} + \frac{77}{72n^4} - \frac{1}{3n^3} + O\left(\frac{1}{n^9}\right)\right) + \sum_{i=1}^{\infty} \frac{1}{\binom{2i}{i} i^3}$$

$$\sum_{i=1}^{n} \frac{\binom{2i}{i}\sum_{j=1}^{i}\frac{1}{j^2}}{i} \sim -\frac{2\zeta_3}{3} + 2^{2n}\sqrt{n}\frac{1}{\sqrt{\pi}}\left(-\frac{2233}{864n^5} - \frac{5}{18n^4} - \frac{4}{3n^3} + \left(\frac{2441}{4608n^5} + \frac{121}{576n^4} + \frac{1}{12n^3} + \frac{2}{9n^2}\right)\pi^2 + O\left(\frac{1}{n^6}\right)\right)$$

All the algorithms mentioned in this talk and many more are implemented in the package

`HarmonicSums`

using `Sigma` for certain subtasks dealing with recurrences and sums.

The packages are available at

http://www.risc.jku.at/research/combinat/software/