

Iterated Binomial Sums and their Associated Iterated Integrals

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LHCphenOnet

- ▶ Iterated Binomial Sums
- ▶ Iterated Integrals over Square-Root Valued Alphabets
- ▶ Mellin Transformation of D-finite Functions
- ▶ Inverse Mellin Transformation
- ▶ Asymptotic Expansions of Nested Sums
- ▶ Generating functions for Iterated Integrals

Nested Sums

$$\sum_{i_1=1}^n s_1(i_1) \sum_{i_2=1}^{i_1} s_2(i_2) \sum_{i_3=1}^{i_2} s_3(i_3) \cdots \sum_{i_k=1}^{i_{k-1}} s_k(i_k)$$

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► $s_i(j) = \frac{(\pm 1)^j}{j^{c_i}}$, $c_i \in \mathbb{N}$

harmonic sums

$$\sum_{i_1=1}^n s_1(i_1) \sum_{i_2=1}^{i_1} s_2(i_2) \sum_{i_3=1}^{i_2} s_3(i_3) \cdots \sum_{i_k=1}^{i_{k-1}} s_k(i_k)$$

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harmonic sums

▶ $s_i(j) = \frac{x_i^j}{j^{c_i}}$, $x_i \in \mathbb{R}^*$; $c_i \in \mathbb{N}$

S-sums

$$\sum_{i_1=1}^n s_1(i_1) \sum_{i_2=1}^{i_1} s_2(i_2) \sum_{i_3=1}^{i_2} s_3(i_3) \cdots \sum_{i_k=1}^{i_{k-1}} s_k(i_k)$$

- ▶ $s_i(j) = \frac{(\pm 1)^j}{j^{c_i}}$, $c_i \in \mathbb{N}$ harmonic sums
- ▶ $s_i(j) = \frac{x_i^j}{j^{c_i}}$, $x_i \in \mathbb{R}^*$; $c_i \in \mathbb{N}$ S-sums
- ▶ $s_i(j) = \frac{(\pm 1)^j}{(a_i j + b_i)^{c_i}}$, $a_i, c_i \in \mathbb{N}$; $b_i \in \mathbb{N}_0$ cyclotomic sums

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- ▶ $s_i(j) = \frac{x_i^j}{j^{c_i}} \binom{2i}{i}^{d_i}$, $x_i \in \mathbb{R}^*$; $c_i \in \mathbb{N}$; $d_i \in \mathbb{Z}$ binomial sums

Definition (Iterated Binomial Sums (B-Sums))

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

$$S_{(a_1, b_1, c_1, d_1, x_1), \dots, (a_k, b_k, c_k, d_k, x_k)}(n) = \sum_{n \geq i_1 \geq \dots \geq i_k \geq 1} \frac{x_1^{i_1}}{(a_1 i_1 + b_1)^{c_1}} \binom{2i_1}{i_1}^{d_1} \cdots \frac{x_k^{i_k}}{(a_k i_k + b_k)^{c_k}} \binom{2i_k}{i_k}^{d_k}$$

k is called the depth and $w = \sum_{i=1}^k c_i$ is called the weight of the iterated binomial sum $S_{(a_1, b_1, c_1, d_1, x_1), \dots, (a_k, b_k, c_k, d_k, x_k)}(n)$.

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$$S_{(2, 1, 3, -1, \frac{1}{4}), (1, 0, 3, 1, 1)}(n) = \sum_{i=1}^n \frac{(\frac{1}{4})^i \sum_{j=1}^i \frac{\binom{2j}{j}}{j^3}}{(2i+1)^3 \binom{2i}{i}}$$

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$$S_{(1, 0, 2, 0, 1), (1, 0, 3, 0, 1), (1, 0, 1, 0, -1)}(n) = \sum_{i=1}^n \frac{\sum_{j=1}^i \frac{\sum_{k=1}^j \frac{(-1)^k}{k}}{j^3}}{i^2}$$

$$S_{\mathbf{p}}(n) S_{\mathbf{q}}(n) = \sum_{\mathbf{r}=\mathbf{p}\sqcup\mathbf{q}} S_{\mathbf{r}}(n) + \text{sums of lower depth}$$

here $\mathbf{p}\sqcup\mathbf{q}$ represent all merges of \mathbf{p} and \mathbf{q} in which the relative orders of the elements of \mathbf{p} and \mathbf{q} are preserved.

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$$\begin{aligned} S_{a_1, a_2}(n) S_{b_1, b_2}(n) &= S_{a_1, a_2, b_1, b_2}(n) + S_{a_1, b_1, a_2, b_2}(n) \\ &\quad + S_{a_1, b_1, b_2, a_2}(n) + S_{b_1, b_2, a_1, a_2}(n) \\ &\quad + S_{b_1, a_1, b_2, a_2}(n) + S_{b_1, a_1, a_2, b_2}(n) \\ &\quad + \text{sums of lower depth} \end{aligned}$$

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

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

$$S_{(1,0,1,1,1)}(n) S_{(2,1,1,1,1),(1,0,2,-1,0)}(n) =$$

$$\begin{aligned}
& S_{(1,0,1,1,1)}(n) S_{(2,1,1,1,1),(1,0,2,-1,0)}(n) = \\
& \quad S_{(2,1,1,1,1),(1,0,2,-1,0),(1,0,1,1,1)}(n) \\
& \quad + S_{(2,1,1,1,1),(1,0,1,1,1),(1,0,2,-1,0)}(n) \\
& \quad + S_{(1,0,1,1,1),(2,1,1,1,1),(1,0,2,-1,0)}(n) \\
& \quad - S_{(1,0,1,1,2),(1,0,2,-1,-1)}(n) \\
& \quad + 2 S_{(2,1,1,1,2),(1,0,2,-1,-1)}(n) \\
& \quad - S_{(2,1,1,1,2),(1,0,3,-1,0)}(n)
\end{aligned}$$

Iterated Integrals

$$\int_0^x f_1(y_1) \int_0^{y_1} f_2(y_2) \int_0^{y_2} f_3(y_3) \cdots \int_0^{y_{k-1}} f_k(y_k) dy_k \cdots dy_3 dy_2 dy_1$$

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- $f_i(y) = \frac{1}{y-a_i}$, $a_i \in \{-1, 0, 1\}$ harmonic polylogarithms

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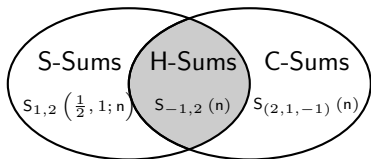
harmonic polylogarithms

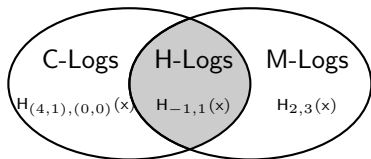
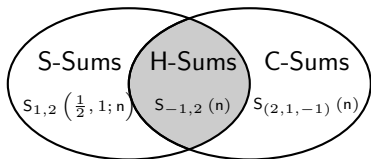
▶ $f_i(y) = \frac{1}{y-a_i}$, $a_i \in \mathbb{R}$

multiple polylogarithms

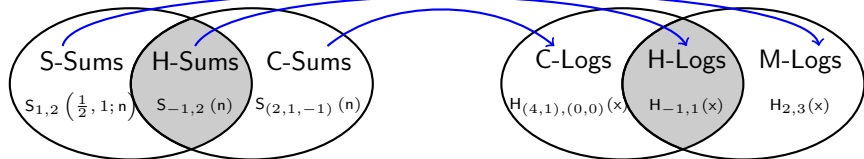
$$\int_0^x f_1(y_1) \int_0^{y_1} f_2(y_2) \int_0^{y_2} f_3(y_3) \cdots \int_0^{y_{k-1}} f_k(y_k) dy_k \cdots dy_3 dy_2 dy_1$$

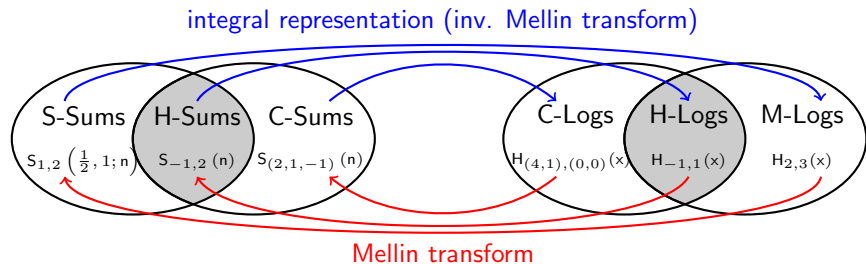
- ▶ $f_i(y) = \frac{1}{y-a_i}$, $a_i \in \{-1, 0, 1\}$ harmonic polylogarithms
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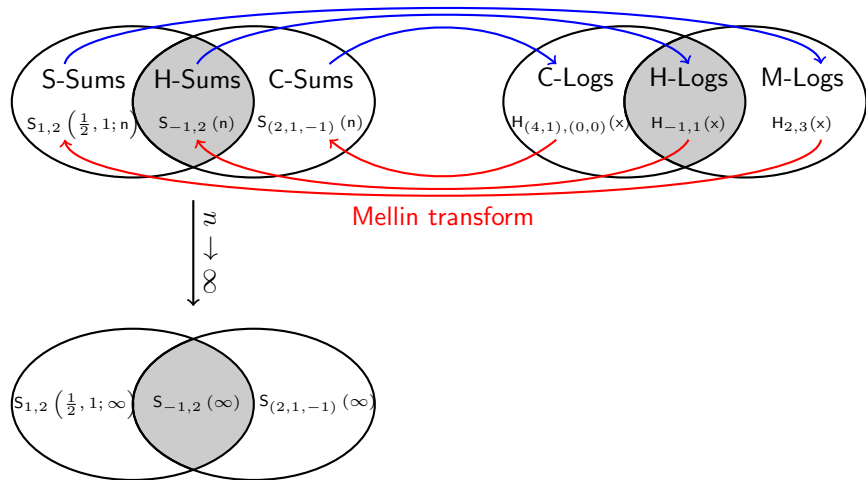


integral representation (inv. Mellin transform)

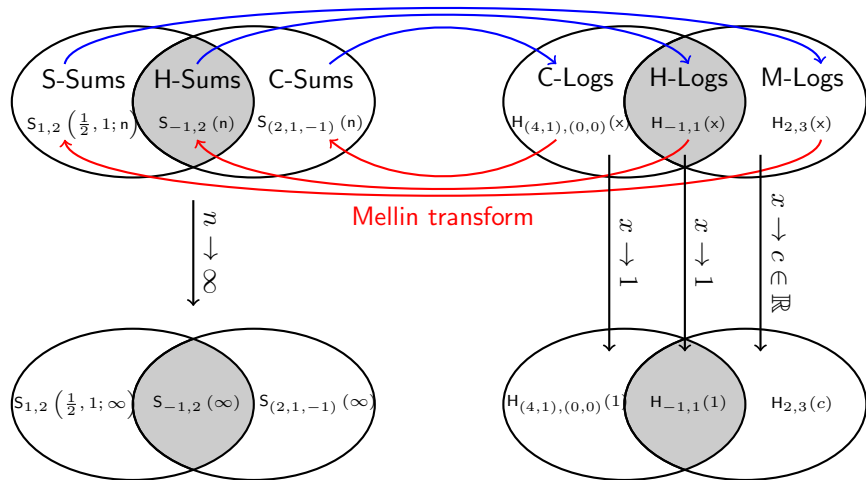




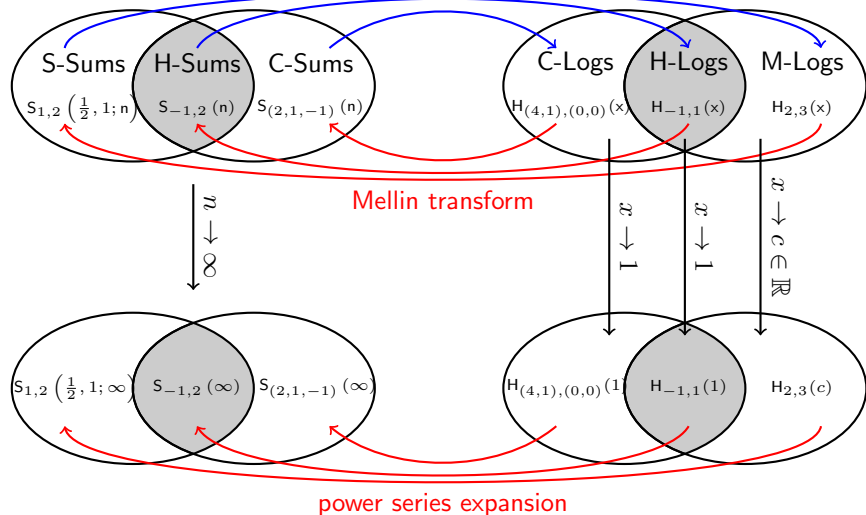
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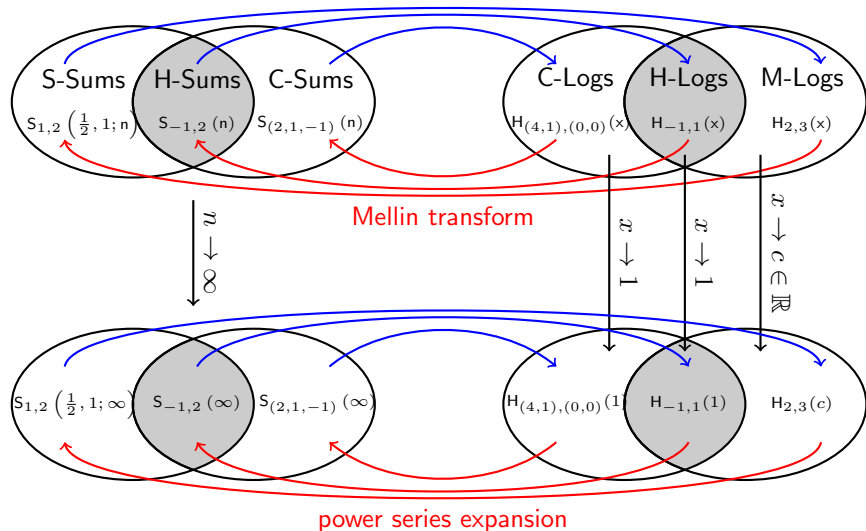
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- ▶ $f_i(y) = \frac{1}{y-a_i}$, $a_i \in \{-1, 0, 1\}$ harmonic polylogarithms
- ▶ $f_i(y) = \frac{1}{y-a_i}$, $a_i \in \mathbb{R}$ multiple polylogarithms
- ▶ $f_i(y) = \frac{y^{j_i}}{\Phi_{a_i}(y)}$, $j_i \in \mathbb{N}$ cyclotomic polylogarithms

$$f_a(x) := \frac{\text{sign}(1 - a - 0)}{x - a},$$

$$f_{\{a_1, \dots, a_k\}}(x) := f_{a_1}(x)^{1/2} \dots f_{a_k}(x)^{1/2} \quad k \geq 2,$$

$$f_{(a_0, \{a_1, \dots, a_k\})}(x) := f_{a_0}(x) f_{a_1}(x)^{1/2} \dots f_{a_k}(x)^{1/2} \quad k \geq 1,$$

$$f_{(\{a_1, \dots, a_k\}, j)}(x) := x^j f_{(a_1, \dots, a_k)}(x) \quad j \in \{1, \dots, k - 2\}.$$

Restricting to at most two root-singularities we are left with the following cases:

$$f_a(x) := \frac{\text{sign}(1 - a - 0)}{x - a},$$

$$f_{(a, \{b\})}(x) := f_a(x) \sqrt{f_b(x)},$$

$$f_{\{a, b\}}(x) := \sqrt{f_a(x)} \sqrt{f_b(x)},$$

$$f_{(a, \{b, c\})}(x) := f_a(x) \sqrt{f_b(x)} \sqrt{f_c(x)}.$$

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$$H_{(2, \{-4\}), (4, \{-1\})}(x) = \int_0^x \frac{1}{(2-x)\sqrt{x+4}} \int_0^y \frac{1}{(4-y)\sqrt{1+y}} dy dx$$

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$$H_{(2), (\{-1\}), (\{-1\})}(x) = \int_0^x \frac{1}{(2-x)} \int_0^y \frac{1}{\sqrt{1+y}} \int_0^y \frac{1}{\sqrt{1+z}} dz dy dx$$

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$$\begin{aligned} H_{a_1,a_2}(x)H_{b_1,b_2}(x) &= H_{a_1,a_2,b_1,b_2}(x) + H_{a_1,b_1,a_2,b_2}(x) \\ &\quad + H_{a_1,b_1,b_2,a_2}(x) + H_{b_1,b_2,a_1,a_2}(x) \\ &\quad + H_{b_1,a_1,b_2,a_2}(x) + H_{b_1,a_1,a_2,b_2}(x) \end{aligned}$$

There are no additional algebraic relations among the iterated integrals if the alphabet is chosen carefully.

Mellin transform

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form a *P-finite* sequence.

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form a P -finite sequence.

- ▶ The generating function of a P -finite sequence $(f_n)_{n \geq 0}$ is D -finite.

- Assume that $f(x) = \sum_{n \geq 0} f_n x^n$ is D-finite such that

$$p_d(x)f^{(d)}(x) + \cdots + p_1(x)f'(x) + p_0(x)f(x) = 0. \quad (1)$$

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- It is easy to check that

$$x^k f^{(j)}(x) = \sum_{n \geq 0} \prod_{i=1}^j (n+i-k) f_{n+j-k} x^n \quad (2)$$

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- ▶ Transform (1) according to this relation.

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

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$$f(x) = \int_0^x \int_0^{\tau_1} \frac{1}{(1 + \tau_1)(1 - \tau_2)} d\tau_2 d\tau_1 = \sum_{n \geq 0} f_n x^n.$$

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$$\begin{aligned} & \sum_{n=0}^{\infty} (n+1)f_{n+1}x^n + 3 \sum_{n=0}^{\infty} n(n+1)f_{n+1}x^n + \sum_{n=0}^{\infty} (n-1)n(n+1)f_{n+1}x^n \\ & - \sum_{n=0}^{\infty} (n+1)(n+2)f_{n+2}x^n - \sum_{n=0}^{\infty} (n+1)(n+2)(n+3)f_{n+3}x^n = 0 \end{aligned}$$

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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 $(f_n)_{n \geq 0}$.

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

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We can conclude:

Proposition

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

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

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Method:

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4. Solve the recurrence to get a closed form representation for $\mathbf{M}[f(x)](n)$.

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

$$\begin{aligned} \mathbf{M}[f(x)](n) &= (-1)^n \left(\frac{4^{n+1}}{(2n+1)(2n+3) \binom{2n}{n}} + \frac{\int_0^1 \frac{\sqrt{1-\tau}}{1+\tau} d\tau - 2}{n+1} \right) \\ &\quad - \frac{4(-1)^n \sum_{i=1}^n \frac{4^i}{(2i+1) \binom{2i}{i}}}{n+1} + \frac{\int_0^1 \frac{\sqrt{1-\tau}}{1+\tau} d\tau}{n+1}. \end{aligned}$$

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$$\int_0^{1-\varepsilon} x^N f(x) dx = \frac{1}{N+1} \left((1-\varepsilon)^{N+1} f(1-\varepsilon) - \int_0^{1-\varepsilon} dx x^{N+1} f'(x) \right)$$

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$$\int_0^{1-\varepsilon} \frac{x^N f(x)}{\sqrt{x-a}} dx = \frac{(4a)^N}{(2N+1) \binom{2N}{N}} \left(\int_0^{1-\varepsilon} dx \frac{f(x)}{\sqrt{x-a}} \right. \\ \left. + 2 \sum_{i=1}^N \frac{\binom{2i}{i}}{(4a)^i} \left(\sqrt{1-a-\varepsilon} (1-\varepsilon)^i f(1-\varepsilon) \right. \right. \\ \left. \left. - \int_0^{1-\varepsilon} dx x^i \sqrt{x-a} f'(x) \right) \right).$$

$$\begin{aligned}
\mathbf{M} \left[H_{h_1, \dots, h_k}^*(x) \right] (N) &= \frac{1}{N+1} \mathbf{M} \left[x h_1(x) H_{h_2, \dots, h_k}^*(x) \right] (N) \\
\mathbf{M} \left[\frac{H_{h_1, \dots, h_k}^*(x)}{\sqrt{x}} \right] (N) &= \frac{1}{N+1/2} \mathbf{M} \left[\sqrt{x} h_1(x) H_{h_2, \dots, h_k}^*(x) \right] (N) \\
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&\quad \left. + 2 \sum_{i=1}^N \frac{\binom{2i}{i}}{(4a)^i} \mathbf{M} \left[\sqrt{x-a} h_1(x) H_{h_2, \dots, h_k}^*(x) \right] (i) \right) \\
\mathbf{M} \left[\frac{H_{h_1, \dots, h_k}^*(x)}{\sqrt{x(x-a)}} \right] (N) &= \left(\frac{a}{4} \right)^N \binom{2N}{N} \left(\int_0^1 dx \frac{H_{h_1, \dots, h_k}^*(x)}{\sqrt{x(x-a)}} + \right. \\
&\quad \left. + \sum_{i=1}^N \frac{(4/a)^i}{i \binom{2i}{i}} \mathbf{M} \left[\sqrt{\frac{x-a}{x}} h_1(x) H_{h_2, \dots, h_k}^*(x) \right] (i) \right)
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- ▶ As a consequence we have the following summation formula

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

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- ▶ Furthermore, the following properties are immediate, where $a > 0$:

$$\mathbf{M} [\ln(x)^m f(x)] (N) = \frac{d^m}{dN^m} \mathbf{M}[f(x)](N),$$

$$\mathbf{M}[f(ax)](N) = \frac{1}{a^{N+1}} \mathbf{M}[f(x)\theta(a-x)](N), \quad a \leq 1,$$

$$\mathbf{M}[f(x^a)](N) = \frac{1}{a} \mathbf{M}[f(x)] \left(\frac{N+1-a}{a} \right) .$$

- ▶ The Mellin-convolution of two real functions is defined by

$$f(x) * g(x) = \int_0^1 dx_1 \int_0^1 dx_2 \delta(x - x_1 x_2) f(x_1) g(x_2) .$$

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- ▶ The Mellin transformation for functions with +-prescription

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

has similar properties.

Inverse Mellin transform

Aim: represent our nested sums in terms of Mellin transforms in the form

$$c_0 + \sum_{j=1}^k c_j^N \mathbf{M}[f_j(x)](N), \quad (3)$$

where the constants c_j and functions $f_j(x)$ do not depend on N .

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- ▶ achieved by virtue of the properties of the Mellin transform.
- ▶ as starting point we only need the following basic integral representations:

$$\begin{aligned} \frac{1}{N} &= \mathbf{M} \left[\frac{1}{x} \right] (N) \\ \binom{2N}{N} &= \frac{4^N}{\pi} \mathbf{M} \left[\frac{1}{\sqrt{x(1-x)}} \right] (N) \\ \frac{1}{N \binom{2N}{N}} &= \frac{1}{4^N} \mathbf{M} \left[\frac{1}{x\sqrt{1-x}} \right] (N). \end{aligned}$$

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we first set up an integral rep. for $a_j(N)$ of the form (3).

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- ▶ By the summation property we obtain an integral representation for (4).
- ▶ Repeat until the outermost sum has been processed.

$$\begin{aligned}
\sum_{i=1}^N \frac{1}{i \binom{2i}{i}} &= \int_0^1 dx \frac{\left(\frac{x}{4}\right)^N - 1}{x - 4} \frac{1}{\sqrt{1-x}} \\
\sum_{i=1}^N \frac{1}{i} \binom{2i}{i} (-1)^i &= \frac{1}{\pi} \int_0^1 dx \frac{(-4x)^N - 1}{x + \frac{1}{4}} H_{w_1}^*(x) \\
\sum_{i=1}^N \frac{1}{i^2 \binom{2i}{i}} \sum_{j=1}^i \binom{2j}{j} (-2)^j &= - \int_0^1 dx \frac{(-2x)^N - 1}{x + \frac{1}{2}} \left(\ln(x) + \frac{H_{w_{28}}^*(x)}{6\sqrt{2}} \right) \\
&\quad - \frac{2}{3} \int_0^1 dx \frac{\left(\frac{x}{4}\right)^N - 1}{x - 4} H_{w_3}^*(x) .
\end{aligned}$$

Asymptotic Expansion of Nested Sums

We say that the function $f : \mathbb{R} \rightarrow \mathbb{R}$ is expanded in an asymptotic series

$$f(x) \sim \sum_{k=0}^{\infty} \frac{a_k}{x^k}, \quad x \rightarrow \infty,$$

where a_k are constants, if for all $K \geq 0$

$$R_K(x) = f(x) - \sum_{k=0}^K \frac{a_k}{x^k} = o\left(\frac{1}{x^K}\right), \quad x \rightarrow \infty.$$

Why do we need these expansions of nested sums?

E.g.,

- ▶ for limits of the form

$$\lim_{n \rightarrow \infty} n \left(S_2(n) - \zeta_2 - S_{2,2}(n) + \frac{7 \zeta_2^2}{10} \right)$$

- ▶ for the approximation of the values of analytic continued nested sums at the complex plane

$$S_{2,-3}(-2.5 + 2i)$$

Basic Idea

$$S_{-1,3}(n) = (-1)^n \int_0^1 x^n \frac{H_{1,0,0}(x)}{1+x} dx + \text{const}$$

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$$\sum_{k=0}^{\infty} \frac{a_{k+1} k!}{n(n+1) \dots (n+k)}$$

Basic Idea

$$\varphi(x) \longrightarrow \varphi(1-x) = \sum_{k=0}^{\infty} a_k x^k$$

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$$+ (-1)^n \left(\frac{1}{2n} - \frac{1}{4n^2} + \frac{1}{8n^4} - \frac{1}{4n^6} \right) \zeta_3 - \frac{19 \zeta_2^2}{40}$$

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Why do we need these expansions of nested sums?

E.g.,

- ▶ for limits of the form

$$\lim_{n \rightarrow \infty} n \left(S_2(n) - \zeta_2 - S_{2,2}(n) + \frac{7 \zeta_2^2}{10} \right) = \zeta_2 - 1$$

- ▶ for the approximation of the values of analytic continued nested sums at the complex plane

$$S_{2,-3}(-2.5 + 2i) = -0.795096 - 0.105476i$$

Generating Functions for Iterated Integrals

Given an iterated integral $f(x)$.

Find a generating series i.e., find $(f_n)_{n \geq 0}$ such that

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- ▶ Solve the recurrence to get a closed form for f_n

Example

We want to compute the power series expansion of

$$f(x) := \int_0^x \frac{\sqrt{1-y}}{1+y} dy.$$

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Computing initial values and solving the recurrence leads to

$$f(x) = \sum_{i=1}^{\infty} (-x)^i \left(\frac{\sum_{j=1}^i \frac{(-\frac{1}{4})^j \binom{2j}{j}}{2^{j-1}}}{i} - \frac{(-\frac{1}{4})^i \binom{2i}{i}}{i(2i-1)} - \frac{1}{i} \right).$$

Nested Sums at Infinity
Iterated Integrals at One

- ▶ Using the generating function we can convert the generalized harmonic polylogarithms at one to binomial sums at infinity.

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- ▶ Relations between the constants due to the shuffle algebra of the iterated integrals.

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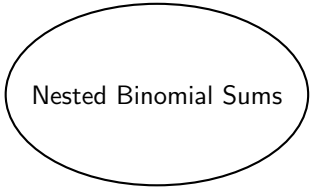
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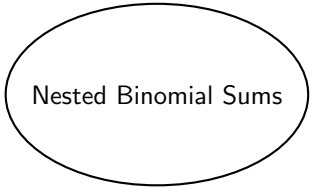
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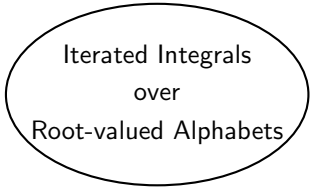
- ▶ Relations between the constants due to the shuffle algebra of the iterated integrals.
- ▶ Relations between the constants due to the quasi shuffle algebra of the nested sums.



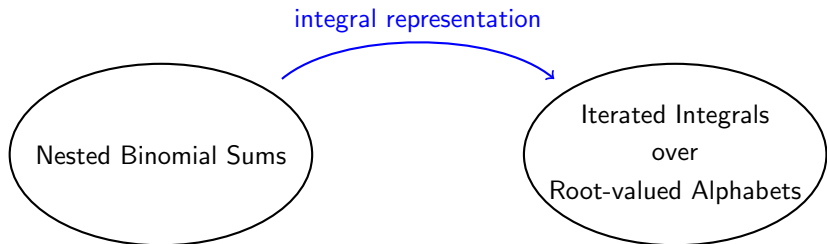
Nested Binomial Sums

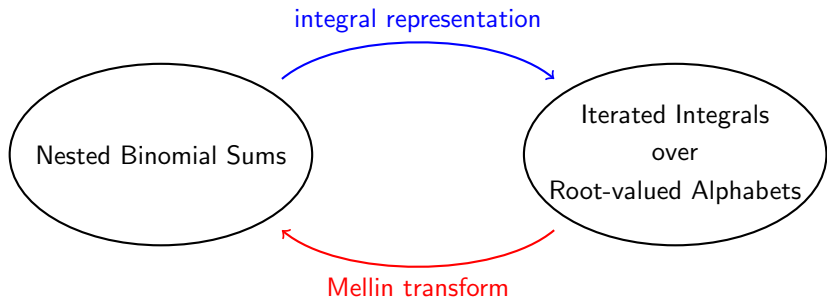


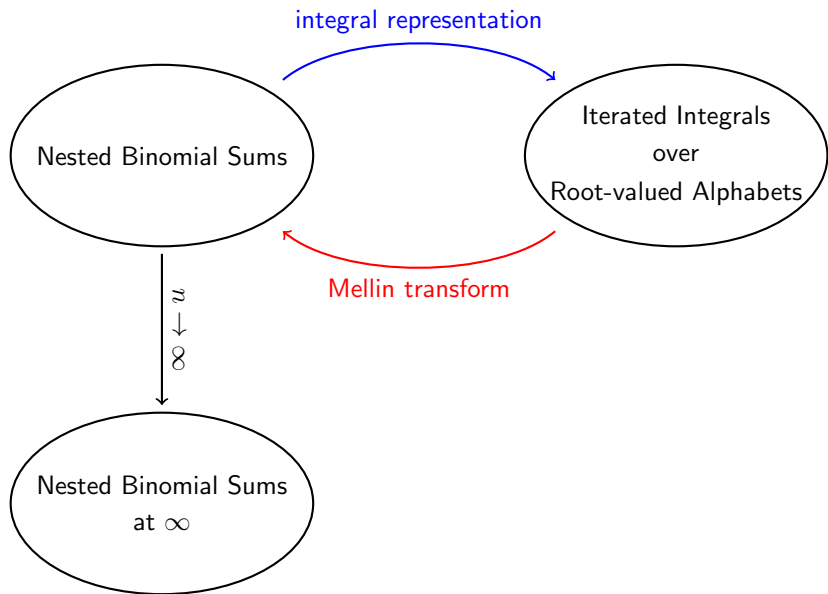
Nested Binomial Sums

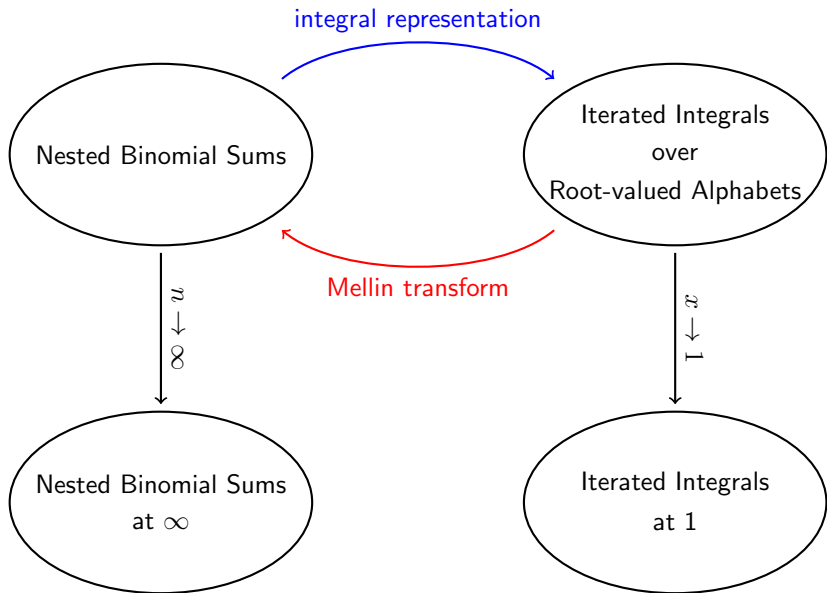


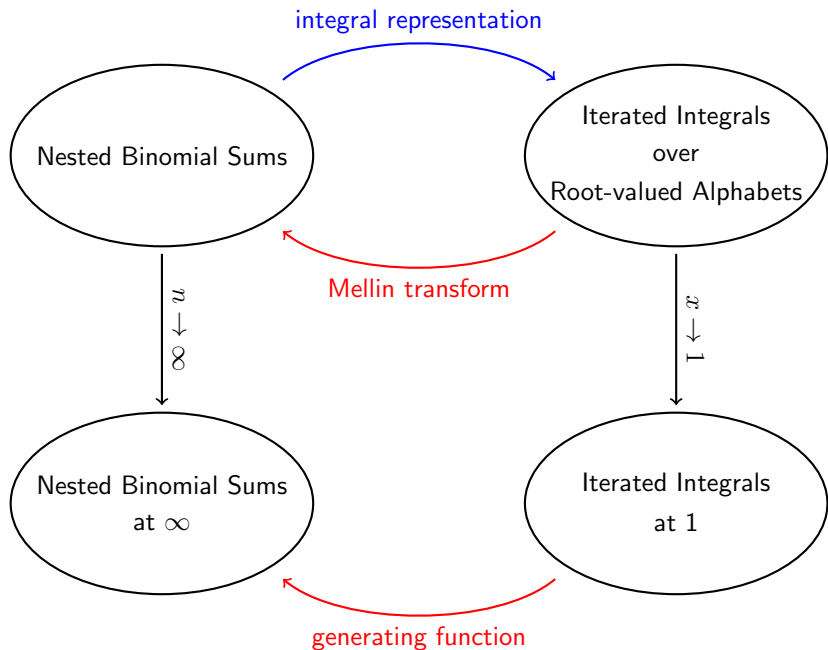
Iterated Integrals
over
Root-valued Alphabets

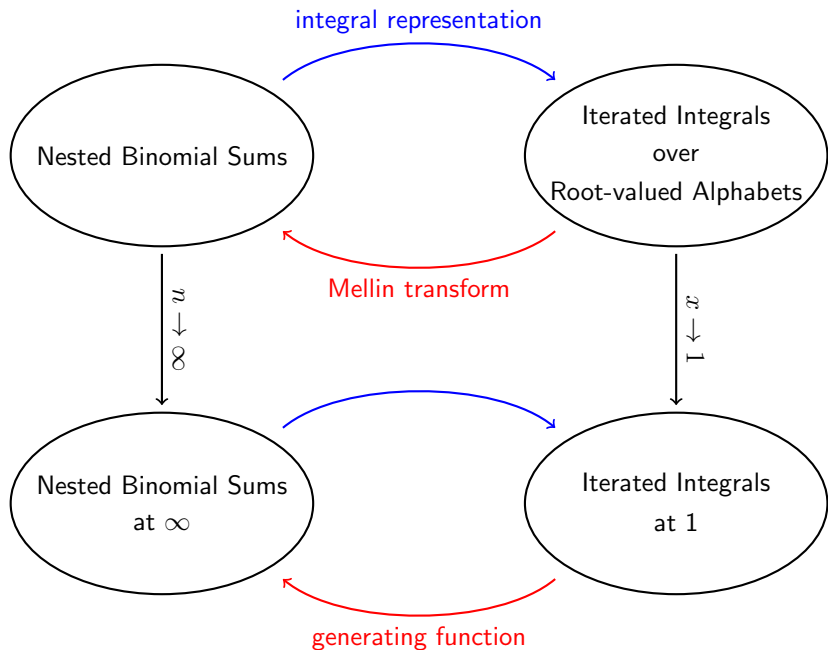












All the algorithms mentioned in this talk and many more are implemented in the package

`HarmonicSums`

which is available at

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