DESY, Zeuthen, Germany

Computer Algebra and Particle Physics - CAPP 2013

Symbolic summation and the Sigma package

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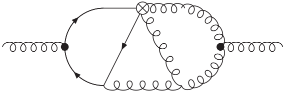
Consider a massive 3–loop ladder graph (Ablinger, Blümlein,Hasselhuhn,Klein, CS,Wißbrock, 2012)



$$= F_{-3}(n)\varepsilon^{-3} + F_{-2}(n)\varepsilon^{-2} + F_{-1}(n)\varepsilon^{-1} + \boxed{F_0(n)}$$

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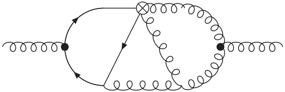

$$= F_{-3}(n)\varepsilon^{-3} + F_{-2}(n)\varepsilon^{-2} + F_{-1}(n)\varepsilon^{-1} + \boxed{F_0(n)}$$

Simplify

$$||$$

$$\sum_{j=0}^{n-3}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{q=0}^{-j+n-3}\sum_{s=1}^{-l+n-q-3}\sum_{r=0}^{-l+n-q-s-3}(-1)^{-j+k-l+n-q-3}\times$$

$$\times\frac{\binom{j+1}{k+1}\binom{k}{l}\binom{n-1}{j+2}\binom{-j+n-3}{q}\binom{-l+n-q-3}{s}\binom{-l+n-q-s-3}{r}r!(-l+n-q-r-s-3)!(s-1)!}{(-l+n-q-2)!(-j+n-1)(n-q-r-s-2)(q+s+1)}$$

$$\Big[4S_1(-j+n-1)-4S_1(-j+n-2)-2S_1(k)$$

$$-(S_1(-l+n-q-2)+S_1(-l+n-q-r-s-3)-2S_1(r+s))$$

$$+2S_1(s-1)-2S_1(r+s)\Big]$$ **+ 3 further 6–fold sums**

$$\boxed{F_0(n)} =$$

$$\frac{7}{12}S_1(n)^4 + \frac{(17n+5)S_1(n)^3}{3n(n+1)} + \Big(\frac{35n^2-2n-5}{2n^2(n+1)^2} + \frac{13S_2(n)}{2} + \frac{5(-1)^n}{2n^2}\Big)S_1(n)^2$$
$$+ \Big(-\frac{4(13n+5)}{n^2(n+1)^2} + \Big(\frac{4(-1)^n(2n+1)}{n(n+1)} - \frac{13}{n}\Big)S_2(n) + \Big(\frac{29}{3} - (-1)^n\Big)S_3(n)$$
$$+ \big(2+2(-1)^n\big)S_{2,1}(n) - 28S_{-2,1}(n) + \frac{20(-1)^n}{n^2(n+1)}\Big)S_1(n) + \Big(\frac{3}{4} + (-1)^n\Big)S_2(n)^2$$
$$- 2(-1)^nS_{-2}(n)^2 + S_{-3}(n)\Big(\frac{2(3n-5)}{n(n+1)} + \big(26+4(-1)^n\big)S_1(n) + \frac{4(-1)^n}{n+1}\Big)$$
$$+ \Big(\frac{(-1)^n(5-3n)}{2n^2(n+1)} - \frac{5}{2n^2}\Big)S_2(n) + S_{-2}(n)\Big(10S_1(n)^2 + \Big(\frac{8(-1)^n(2n+1)}{n(n+1)}$$
$$+ \frac{4(3n-1)}{n(n+1)}\Big)S_1(n) + \frac{8(-1)^n(3n+1)}{n(n+1)^2} + \big(-22+6(-1)^n\big)S_2(n) - \frac{16}{n(n+1)}\Big)$$
$$+ \Big(\frac{(-1)^n(9n+5)}{n(n+1)} - \frac{29}{3n}\Big)S_3(n) + \Big(\frac{19}{2} - 2(-1)^n\Big)S_4(n) + \big(-6+5(-1)^n\big)S_{-4}(n)$$
$$+ \Big(-\frac{2(-1)^n(9n+5)}{n(n+1)} - \frac{2}{n}\Big)S_{2,1}(n) + \big(20+2(-1)^n\big)S_{2,-2}(n) + \big(-17+13(-1)^n\big)S_{3,1}(n)$$
$$- \frac{8(-1)^n(2n+1)+4(9n+1)}{n(n+1)}S_{-2,1}(n) - \big(24+4(-1)^n\big)S_{-3,1}(n) + \big(3-5(-1)^n\big)S_{2,1,1}(n)$$
$$+ 32S_{-2,1,1}(n) + \left(\frac{3}{2}S_1(n)^2 - \frac{3S_1(n)}{n} + \frac{3}{2}(-1)^nS_{-2}(n)\right)\zeta(2)$$

Some literature (for users)

- For hypergeometric sequences:

  $A = B$, M. Petkovšek, H. S. Wilf, and D. Zeilberger, 1996. Available at http://www.math.upenn.edu/∼wilf/AeqB.html

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  C. Schneider. Simplifying Multiple Sums in Difference Fields. *Available this April, 2013.*

Part 1: Indefinite summation

Simplify

$$\sum_{k=1}^{n} S_1(k) = \text{?}$$

where $S_1(k) = \sum_{i=1}^{k} \frac{1}{i}$

Software

Telescoping

GIVEN $f(k) = S_1(k)$.

FIND $g(k)$:

$$\boxed{f(k) = g(k+1) - g(k)}$$

for all $1 \leq k \leq n$ and $n \geq 0$.

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We compute

$$g(k) = (S_1(k) - 1)k.$$

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Summing this equation over k from 1 to n gives

$$\boxed{\sum_{k=1}^{n} S_1(k)} = \boxed{g(n+1) - g(1)}$$

$$= (S_1(n+1) - 1)(n+1).$$

$$\sum_{k=0}^{a} F(k) = ?$$

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Indefinite summation.
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`SigmaReduce[`$\sum_{k=0}^{a} F(k)$`]`

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$$\frac{k \cdot k + 2 \cdot k - \zeta_2}{(k+1)(k+2)}$$

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$$\sum_{i=l}^{k} f(i) \quad \text{or} \quad \prod_{i=l}^{k} f(i) \qquad l \in \mathbb{N}$$

$f(i)$: free of k and nested product-sum expression w.r.t. i.

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$$\sum_{j=1}^{k} \frac{\left(\sum_{i=1}^{j} \frac{1}{i}\right)^2}{\sum_{i=1}^{j} \frac{1}{(i^2+1)} + \prod_{i=1}^{j} \sum_{r=1}^{i} \frac{1}{r}}$$

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$+,\ -,\ *,\ /,$ `SigmaSum[f,{i,l,k}]` `SigmaProduct[f,{i,l,k}]`

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Telescoping in the given difference field

FIND a closed form for

$$\sum_{k=1}^{n} S_1(k).$$

A difference field for the summand

Consider the rational function field

$$\mathbb{F} := \mathbb{Q}$$

with the automorphism $\sigma : \mathbb{F} \to \mathbb{F}$ defined by

$$\sigma(c) = c \quad \forall c \in \mathbb{Q},$$

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$$\sigma(h) = h + \frac{1}{k+1}, \qquad \mathcal{S}\, S_1(k) = S_1(k) + \frac{1}{k+1}.$$

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FIND $g \in \mathbb{F}$:

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with

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$$g(k) = (S_1(k) - 1)k.$$

Hence,

$$(S_1(n+1) - 1)(n+1) = \sum_{k=1}^{n} S_1(k).$$

The basic summation algorithm

(a simplified version of Karr's algorithm, 1981)

CONSTRUCT a difference field $(\mathbb{F}, \sigma)$:

- a rational function field

$$\mathbb{F} := \mathbb{K}$$

- with an automorphism

$$\sigma(c) = c \quad \forall c \in \mathbb{K}$$

CONSTRUCT a difference field $(\mathbb{F}, \sigma)$:

- a rational function field

$$\mathbb{F} := \mathbb{K}(t_1)$$

- with an automorphism

$$\sigma(c) = c \quad \forall c \in \mathbb{K}$$
$$\sigma(t_1) = a_1\, t_1 + f_1, \quad a_1 \in \mathbb{K}^*, \qquad f_1 \in \mathbb{K}$$

CONSTRUCT a difference field $(\mathbb{F}, \sigma)$:

- a rational function field

$$\mathbb{F} := \mathbb{K}(t_1)(t_2)$$

- with an automorphism

$$\begin{aligned} \sigma(c) &= c \quad \forall c \in \mathbb{K} \\ \sigma(t_1) &= a_1\, t_1 + f_1, \quad a_1 \in \mathbb{K}^*, \qquad f_1 \in \mathbb{K} \\ \sigma(t_2) &= a_2\, t_2 + f_2, \quad a_2 \in \mathbb{K}(t_1)^*, \qquad f_2 \in \mathbb{K}(t_1) \end{aligned}$$

CONSTRUCT a difference field $(\mathbb{F}, \sigma)$:

- a rational function field

$$\mathbb{F} := \mathbb{K}(t_1)(t_2)\dots(t_e)$$

- with an automorphism

$$\begin{aligned}
\sigma(c) &= c \quad \forall c \in \mathbb{K} \\
\sigma(t_1) &= a_1\, t_1 + f_1, \quad a_1 \in \mathbb{K}^*, && f_1 \in \mathbb{K} \\
\sigma(t_2) &= a_2\, t_2 + f_2, \quad a_2 \in \mathbb{K}(t_1)^*, && f_2 \in \mathbb{K}(t_1) \\
&\vdots \\
\sigma(t_e) &= a_e\, t_e + f_e, \quad a_e \in \mathbb{K}(t_1, \dots, t_{e-1})^*, && f_e \in \mathbb{K}(t_1, \dots, t_{e-1})
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\end{aligned}$$

GIVEN $f \in \mathbb{F}$;
FIND $g \in \mathbb{F}$ such that

$$\sigma(g) - g = f.$$

CONSTRUCT a $\Pi\Sigma$-field $(\mathbb{F},\sigma)$:

- a rational function field

$$\mathbb{F} := \mathbb{K}(t_1)(t_2)\dots(t_e)$$

- with an automorphism

$$\begin{aligned}
\sigma(c) &= c \quad \forall c \in \mathbb{K} \\
\sigma(t_1) &= a_1\, t_1 + f_1, \quad a_1 \in \mathbb{K}^*, && f_1 \in \mathbb{K} \\
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\end{aligned}$$

such that

$$\text{const}_\sigma\mathbb{F} = \{c \in \mathbb{K}(t_1)(t_2)\dots(t_e) | \sigma(c) = c\} = \mathbb{K}.$$

GIVEN $f \in \mathbb{F}$;
FIND $g \in \mathbb{F}$ such that

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Telescoping in the given difference field

FIND a closed form for

$$\sum_{k=1}^{n} S_1(k).$$

A $\Pi\Sigma^*$-field for the summand

$$\boxed{\text{const}_\sigma \mathbb{F} = \mathbb{Q}}$$

Consider the rational function field

$$\mathbb{F} := \mathbb{Q}(k)(h)$$

with the automorphism $\sigma : \mathbb{F} \to \mathbb{F}$ defined by

$$\begin{aligned} \sigma(c) &= c \quad \forall c \in \mathbb{Q}, \\ \sigma(k) &= k + 1, & \mathcal{S}\, k &= k + 1, \\ \sigma(h) &= h + \frac{1}{k+1}, & \mathcal{S}\, S_1(k) &= S_1(k) + \frac{1}{k+1}. \end{aligned}$$

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Denominator bound: COMPUTE a polynomial $d \in \mathbb{Q}(k)[h]^*$:

$d = 1$

$$\forall g \in \mathbb{Q}(k)(h): \quad \sigma(g) - g = h \quad \Rightarrow \quad g\,d \in \mathbb{Q}(k)[h].$$

FIND $g' \in \mathbb{Q}(k)[h]$ with

$$\sigma\left(\frac{g'}{d}\right) - \frac{g'}{d} = h.$$

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$$\sigma(\frac{g'}{d}) - \frac{g'}{d} = h.$$

Degree bound: COMPUTE $b \geq 0$:

$$b = 2$$

$$\forall g \in \mathbb{Q}(k)[h] \quad \sigma(g) - g = h \quad \Rightarrow \quad \deg(g) \leq b.$$

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Polynomial Solution: FIND

g=hk-k

$$g = g_2\,h^2 + g_1\,h + g_0 \in \mathbb{Q}(k)[h].$$

ANSATZ $g = g_2\, h^2 + g_1\, h + g_0 \in \mathbb{Q}(k)[h]$

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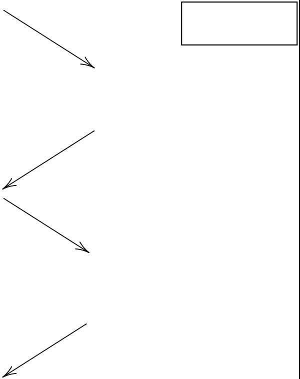

ANSATZ $g = g_2\, h^2 + g_1\, h + g_0 \in \mathbb{Q}(k)[h]$

$$\left[\sigma(g_2)\left(h+\tfrac{1}{k+1}\right)^2+\sigma(g_1 h+g_0)\right] -\left[g_2\, h^2 + g_1 h + g_0\right] = h$$

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coeff. comp.

$\sigma(g_2) - g_2 = 0$

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coeff. comp.

$$\sigma(g_2) - g_2 = 0$$

$g_2 = c \in \mathbb{Q}$

$$\sigma(g_1\, h + g_0) - (g_1\, h + g_0) = h - c\left[\tfrac{2h(k+1)+1}{(k+1)^2}\right]$$

ANSATZ $g = g_2\,h^2 + g_1\,h + g_0 \in \mathbb{Q}(k)[h]$

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$\leftarrow$ $g_0 = -k$, $d = 0$

Difference equations in difference fields

Let $(\mathbb{F}, \sigma)$ be a $\Pi\Sigma$-field with constant field $\mathbb{K}$

Telescoping

- Given $f \in \mathbb{F}$.
- Find $g \in \mathbb{F}$:

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Parameterized first order difference equation

- Given $f_0, \dots, f_d \in \mathbb{F}$, $a_0, a_1 \in \mathbb{F}$.
- Find all $c_0, \dots, c_d \in \mathbb{K}$, $g \in \mathbb{F}$:

$$\boxed{a_1\, \sigma(g) + a_0\, g = c_0\, f_0 + \dots + c_d\, f_d.}$$

Simplification in $\Pi\Sigma$-fields

A difference field approach (M. Karr, 1981)

GIVEN a $\Pi\Sigma$-field $(\mathbb{F}, \sigma)$ with $f \in \mathbb{F}$.

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appropriate = degrees in denominators minimal

Example

$$\sum_{k=1}^{a}\Big(\frac{-2+k}{10(1+k^2)}+\frac{(1-4k-2k^2)S_1(k)}{10(1+k^2)(2+2k+k^2)}+\frac{(1-4k-2k^2)S_3(k)}{5(1+k^2)(2+2k+k^2)}\Big)$$

$$=\frac{a^2+4a+5}{10(a^2+2a+2)}S_1(a)-\frac{(a-1)(a+1)}{5(a^2+2a+2)}S_3(a)-\frac{2}{5}\sum_{k=1}^{a}\frac{1}{k^2}$$

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appropriate = sum representations with optimal nesting depth

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

depth 3 depth 1

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$\Pi\Sigma$-field $(\mathbb{Q}(k)(h),\sigma)$ with

$$\sigma(k)=k+1$$

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$\Pi\Sigma$-field $(\mathbb{Q}(k)(h)(s),\sigma)$ with

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$$\sum_{k=1}^{n} \frac{\sum_{j=1}^{k} \frac{\sum_{i=1}^{j} \frac{1}{i}}{j}}{k} \qquad t$$

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No simplification

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appropriate = sum representations with minimal number of objects Example

$$\sum_{k=0}^{a}(-1)^k S_1(k)^2\binom{n}{k}$$
$$=-\frac{1}{n}\sum_{i_1=1}^{a}\frac{(-1)^{i_1}}{i_1}\binom{n}{i_1}-(a-n)\big(n^2S_1(a)^2+2nS_1(a)+2\big)\frac{(-1)^a\binom{n}{a}}{n^3}-\frac{2}{n^2}$$

Simplification of nested product-sum expressions

$A(k)$: nested product-sum expression (sums/products not in the denominator)

$\downarrow$ `SigmaReduce[A,k]`

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Examples

Constructing $\Pi\Sigma$-fields

CONSTRUCT a $\Pi\Sigma$-field $(\mathbb{F}, \sigma)$:

- a rational function field

$$\mathbb{F} := \mathbb{K}$$

- with an automorphism

$$\sigma(c) = c \quad \forall c \in \mathbb{K}$$

such that

$$\text{const}_\sigma \mathbb{F} = \{c \in \mathbb{K} \quad | \sigma(c) = c\} = \mathbb{K}.$$

CONSTRUCT a $\Pi\Sigma$-field $(\mathbb{F},\sigma)$:

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$$\mathbb{F} := \mathbb{K}(t_1)$$

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$$\sigma(c) = c \quad \forall c \in \mathbb{K}$$
$$\sigma(t_1) = a_1\, t_1 + f_1, \quad a_1 \in \mathbb{K}^*, \qquad f_1 \in \mathbb{K}$$

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Construction of Σ^*-extensions

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Such a difference field extension $(\mathbb{F}(t), \sigma)$ of $(\mathbb{F}, \sigma)$ is called Σ^*-extension

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1. $\boxed{\nexists g \in \mathbb{F} : \ \sigma(g) = g + f}$ $(\mathbb{F}(t), \sigma)$ is a Σ^*-extension of $(\mathbb{F}, \sigma)$
2. $\boxed{\exists g \in \mathbb{F} : \sigma(g) = g + f}$ No need for a Σ^*-extension!