

RISC/SCIENCE Training School in Symbolic Computation 2010

Sigma - A package for multi-summation

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Some literature

- ▶ For hypergeometric terms:

R.W. Gosper. *Decision procedures for indefinite hypergeometric summation*, Proc. Nat. Acad. Sci. U.S.A.", pp 40-42, 1978.

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

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M. Karr. Summation in finite terms. *J. ACM*, 28:305–350, 1981.

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- ▶ For difference fields:

M. Karr. Summation in finite terms. *J. ACM*, 28:305–350, 1981.

C. Schneider. Symbolic summation assists combinatorics. *Sém. Lothar. Combin.*, 56:1–35, 2007. Available at <http://www.mat.univie.ac.at/~slc/>

Warmup example

FIND a closed form for

$$\sum_{k=1}^n H_k = ? ,$$

where $H_n := \sum_{k=1}^n \frac{1}{k}$.

Telescoping

GIVEN $f(k) = H_k$.

FIND $g(k)$:

$$f(k) = g(k+1) - g(k)$$

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

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Sigma computes

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

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Summing this equation over k from 1 to n gives

$$\begin{aligned} \sum_{k=1}^n H_k &= g(n+1) - g(1) \\ &= (H_{n+1} - 1)(n+1). \end{aligned}$$

Telescoping

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$$\sum_{k=1}^n H_k = g(n + 1) - g(1) \\ = (H_{n+1} - 1)(n + 1).$$

Try it out!

Telescoping

FIND a closed form for

$$\sum_{k=1}^n H_k.$$

A difference field for the **summand**

Consider the rational function field

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

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

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

Telescoping

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A difference field for the summand

Consider the rational function field

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

$$S k = k + 1,$$

Telescoping

FIND a closed form for

$$\sum_{k=1}^n H_k.$$

A difference field for the summand

Consider the rational function field

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

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

$$\sigma(h) = h + \frac{1}{k+1},$$

$$S k = k + 1,$$

$$S H_k = H_k + \frac{1}{k+1}.$$

Telescoping in the given difference field

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

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

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with

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Hence,

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

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Denominator bound: COMPUTE a polynomial $0 \neq d \in \mathbb{Q}(k)[h]$:

$$d = 1$$

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

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

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

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Degree bound: COMPUTE $b \geq 0$:

$$b = 2$$

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

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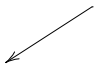
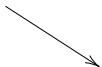
Polynomial Solution: FIND

$$g = hk - k$$

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

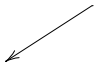
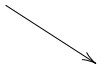
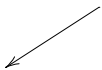
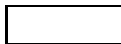
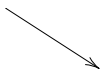
ANSATZ $g = g_2 h^2 + g_1 h + g_0 \in \mathbb{Q}(k)[h]$

$$\sigma(g) - g = h$$



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



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The general case (Karr's algorithm)

GIVEN a $\Pi\Sigma$ -field (\mathbb{F}, σ) :

a rational function field $\mathbb{F} := \mathbb{K}(t_1)(t_2) \dots (t_e)$ with an automorphism

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such that $\{c \in \mathbb{K}(t_1) \dots (t_e) \mid \sigma(c) = c\} = \mathbb{K}$.

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GIVEN $f \in \mathbb{F}$;

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

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

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GIVEN $f \in \mathbb{F}$; (For refined versions see below)

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

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

telescoping

- ▶ GIVEN

$$\sum_{k=0}^n f(k).$$

- ▶ FIND $g(k)$:

$$f(k) = g(k+1) - g(k)$$

telescoping

- ▶ GIVEN

$$\sum_{k=0}^n f(k).$$

- ▶ FIND $g(k)$:

$$f(k) = g(k+1) - g(k)$$

- ▶ THEN (with some mild extra conditions)

$$\sum_{k=0}^n f(k) = g(n+1) - g(0)$$

Refined telescoping

- ▶ GIVEN

$$\sum_{k=0}^n f(k).$$

- ▶ FIND $g(k)$ and $f^*(k)$:

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

where $f^*(k)$ is simpler than $f(k)$.

- ▶ THEN (with some mild extra conditions)

$$\sum_{k=0}^n f(k) = g(n+1) - g(0) + \sum_{k=0}^n f^*(k).$$

Degree optimal w.r.t the top extension

$$\sum_{k=1}^n \frac{1}{k(k+1)^2(k+2)^3} =$$

$$\sum_{k=2}^n \frac{2 - kH_k + H_k^4 - kH_k^5}{H_k - kH_k^2} =$$

Sigma

$$\sum_{k=1}^n H_k^4 =$$

Degree optimal w.r.t the top extension

$$\begin{aligned}
\sum_{k=1}^n \frac{1}{k(k+1)^2(k+2)^3} &= -\frac{1}{4} \sum_{k=1}^n \frac{9k+2}{k^3} \\
&+ \frac{n(69n^5 + 585n^4 + 1967n^3 + 3283n^2 + 2728n + 904)}{16(n+1)^3(n+2)^3} \\
\sum_{k=2}^n \frac{2 - kH_k + H_k^4 - kH_k^5}{H_k - kH_k^2} &= \sum_{k=2}^n \frac{k^2 + H_k}{k^2 H_k} \\
&+ (n+1)H_n^3 - (2n+1)\left(\frac{3}{2}H_n^2 - 3H_n + \frac{3}{2}\right) + \frac{1}{H_n} \\
\sum_{k=1}^n H_k^4 &= -H_n^{(3)} - 2H_n^{(2)} + 2 \sum_{k=1}^n \frac{H_k}{k^2} \\
&+ (n+1)H_n^4 - 2(2n+1)H_n^3 + 6(2n+1)H_n^2 - 12(2n+1)H_n + 24n.
\end{aligned}$$

Simpler w.r.t. the depth

$$\sum_{k=1}^n H_k^2 H_k^{(2)} =$$
$$\sum_{k=0}^a \left(\sum_{i=0}^k \binom{n}{i} \right)^2 =$$
$$\sum_{k=1}^n \frac{\sum_{j=1}^k \frac{H_j}{j^2}}{k^3} =$$

Sigma

Simpler w.r.t. the depth

$$\sum_{k=1}^n H_k^2 H_k^{(2)} = \frac{1}{3} H_n^{(3)} - \frac{1}{3} H_n^3 + \left((n+1) H_n^{(2)} + 1 \right) H_n^2 + (2n+1) (1 - H_n) H_n^{(2)} - 2H_n$$

$$\sum_{k=0}^a \left(\sum_{i=0}^k \binom{n}{i} \right)^2 = (n-a) \binom{n}{a} \sum_{i=0}^a \binom{n}{i} - \frac{n-2a-2}{2} \left(\sum_{i=0}^a \binom{n}{i} \right)^2 - \frac{n}{2} \sum_{i=1}^a \binom{n}{i}^2$$

$$\sum_{k=1}^n \frac{\sum_{j=1}^k \frac{H_j}{j^2}}{k^3} =$$

$$= H_n^{(3)} \sum_{j=1}^n \frac{H_j}{j^2} - \sum_{j=1}^n \frac{H_j H_j^{(3)}}{j^2} + \sum_{j=1}^n \frac{H_j}{j^5}$$

Simpler w.r.t. the depth

$$\sum_{k=1}^n H_k^2 H_k^{(2)} = \frac{1}{3} H_n^{(3)} - \frac{1}{3} H_n^3 + \left((n+1) H_n^{(2)} + 1 \right) H_n^2 + (2n+1) (1 - H_n) H_n^{(2)} - 2H_n$$

$$\sum_{k=0}^a \left(\sum_{i=0}^k \binom{n}{i} \right)^2 = (n-a) \binom{n}{a} \sum_{i=0}^a \binom{n}{i} - \frac{n-2a-2}{2} \left(\sum_{i=0}^a \binom{n}{i} \right)^2 - \frac{n}{2} \sum_{i=1}^a \binom{n}{i}^2$$

$$\sum_{k=1}^n \frac{\sum_{j=1}^k \frac{H_j}{j^2}}{k^3} = S(3, 2, 1, N) \quad (\text{Harmonic sum})$$

$$= H_n^{(3)} \sum_{j=1}^n \frac{H_j}{j^2} - \sum_{j=1}^n \frac{H_j H_j^{(3)}}{j^2} + \sum_{j=1}^n \frac{H_j}{j^5} \quad (\text{Euler sums})$$

Further examples

$$\sum_{k=1}^n H_k^3 = \frac{1}{2} \left(2(n+1)H_n^3 - 3(2n+1)H_n^2 + 6(2n+1)H_n - 12n - 1 + H_n^{(2)} \right)$$

$$\sum_{k=1}^n \frac{1}{k} \sum_{j=1}^k \frac{1}{j} \sum_{i=1}^j \frac{1}{i} = \frac{1}{6} [H_n^3 + 3H_n H_n^{(2)} + 2H_n^{(3)}]$$

$$\begin{aligned} \sum_{k=1}^n \left(\sum_{j=1}^k \frac{H_j^{(2)}}{j^3} \right)^2 &= - (H_n^{(2)})^2 + H_n^{(4)} \sum_{j=1}^n \frac{H_j^{(2)}}{j^3} + (n+1) \left(\sum_{j=1}^n \frac{H_j^{(2)}}{j^3} \right)^2 \\ &\quad + \sum_{j=1}^n \frac{H_j^{(2)3}}{j^3} - \sum_{j=1}^n \frac{H_j^{(2)2}}{j^5} + \sum_{j=1}^n \frac{H_j^{(2)} H_j^{(4)}}{j^3}. \end{aligned}$$

telescoping

GIVEN

$$S(n) = \sum_{k=0}^n \overbrace{\binom{n}{k} H_n}^{=: f(n, k)} .$$

FIND $g(n, k)$:

$$g(n, k + 1) - g(n, k) = f(n, k)$$

no solution 

Creative telescoping

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$$S(n) = \sum_{k=0}^n \overbrace{\binom{n}{k} H_n}^{=: f(n, k)} .$$

FIND $g(n, k)$ and $c_0(n), c_1(n)$:

$$g(n, k + 1) - g(n, k) = c_0(n)f(n, k) + c_1(n)f(n + 1, k)$$

no solution 😞

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$$g(n, k+1) - g(n, k) = c_0(n)f(n, k) + c_1(n)f(n+1, k) + c_2(n)f(n+2, k).$$

Sigma computes:

$$c_0(n) := 4(1+n), \quad c_1(n) := -2(3+2n), \quad c_2(n) := 2+n,$$

$$g(n, k) := \frac{(1+n)(-2+k-n+(2k-2k^2+kn)H_k) \binom{n}{k}}{(1-k+n)(2-k+n)}.$$

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$$g(n, k+1) - g(n, k) = c_0(n)f(n, k) + c_1(n)f(n+1, k) + c_2(n)f(n+2, k).$$

Summing this equation over k from 0 to n gives:

$$\begin{aligned} g(n, n+1) - g(n, 0) = & c_0(n) S(n) + \\ & c_1(n) \left[S(n+1) - f(n+1, n+1) \right] + \\ & c_2(n) \left[S(n+2) - f(n+2, n+1) - f(n+2, n+2) \right] \end{aligned}$$

FIND a recurrence for

$$S(n) := \sum_{k=1}^n \binom{n}{k} H_k.$$

A difference field for the **summand**

Consider the rational function field

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

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

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

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

$$\sigma(h) = h + \frac{1}{k+1},$$

$$\sigma(b) = \frac{n-k}{k+1} b,$$

$$S k = k + 1,$$

$$S H_k = H_k + \frac{1}{k+1},$$

$$S \binom{n}{k} = \frac{n-k}{k+1} \binom{n}{k}.$$

REPRESENT $f(n+i, k)$ in \mathbb{F} :

$$f(n, k) = \mathbf{H}_k \binom{n}{k} \longleftrightarrow hb =: f_0$$

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FIND $c_0, c_1, c_2 \in \mathbb{Q}(n)$ and $g \in \mathbb{F}$:

$$\sigma(g) - g = c_0 f_0 + c_1 f_1 + c_2 f_2.$$

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This gives

$$g(n, k+1) - g(n, k) = c_0(n)f(n, k) + c_1(n)f(n+1, k) + c_2(n)f(n+2, k)$$

with

$$c_0(n) := 4(1+n), \quad c_1(n) := -2(3+2n), \quad c_2(n) := 2+n,$$

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Summing over k from 0 to n gives

$$1 = 4(1+n)S(n) - 2(3+2n)S(n+1) + (2+n)S(n+2)$$

for

$$S(n) = \sum_{k=0}^n \binom{n}{k} H_k.$$

Sigma

1. Creative telescoping (for the special case of hypergeometric terms see Zeilberger's algorithm (1991))

GIVEN a definite sum

$$S(n) = \sum_{k=0}^n f(n, k);$$

$f(n, k)$: indefinite nested product-sum in k ;
 n : extra parameter

FIND a recurrence for $S(n)$

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$$a_0(n), \dots, a_d(n), h(n):$$

indefinite nested product-sum expressions.

$$a_0(n)S(n) + \dots + a_d(n)S(n+d) = h(n);$$

FIND **all solutions** expressible by indefinite nested products and sums

(Nörlund 24, Petkovšek 92, Abramov/Petkovšek 94, Hendriks/Singer 99/Sigma 01)

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NOTE: By construction, the solutions are highly nested.

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3. Indefinite summation (by Sigma's refined summation theory of $\Pi\Sigma^*$ -fields)

Simplify the solutions:

- ▶ The sums have **minimal nested depth**.
- ▶ **No algebraic relations** occur among the sums.

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4. Find a “closed form”

S(n)=combined solutions.

Real life problem: Simplify $f(N, k, j)$

$$\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \left(\frac{(2j+k+N+2)j!k!(j+k+N)!}{(j+k+1)(j+N+1)(j+k+1)!(j+N+1)!(k+N+1)!} \right) + \frac{j!k!(j+k+N)!(-H_j + H_{j+k} + H_{j+N} - H_{j+k+N})}{(j+k+1)!(j+N+1)!(k+N+1)!}$$

where

$$H_N = \sum_{i=1}^N \frac{1}{i}$$

Arose in the context of

I. Bierenbaum, J. Blümlein, and S. Klein, *Evaluating two-loop massive operator matrix elements with Mellin-Barnes integrals*. 2006

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$$f(N, k, j) = g(j+1) - g(j)$$

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$$g(j) = \frac{(j+k+1)(j+N+1)j!k!(j+k+N)!(H_j - H_{j+k} - H_{j+N} + H_{j+k+N})}{kN(j+k+1)!(j+N+1)!(k+N+1)!}$$

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Summing the telescoping equation over j from 0 to a gives

$$\sum_{j=0}^a f(N, k, j) = g(a+1) - g(0)$$

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$$\sum_{j=0}^a f(N, k, j) = \frac{(a+1)!(k-1)!(a+k+N+1)!(H_a - H_{a+k} - H_{a+N} + H_{a+k+N})}{N(a+k+1)!(a+N+1)!(k+N+1)!} \\ + \frac{H_k + H_N - H_{k+N}}{kN(k+N+1)N!} + \frac{(2a+k+N+2)a!k!(a+k+N)!}{(a+k+1)(a+N+1)(a+k+1)!(a+N+1)!(k+N+1)!}$$

$a \rightarrow \infty$

Real life problem: Simplify $f(N, k, j)$

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$$\sum_{j=0}^{\infty} f(N, k, j) = \frac{H_k + H_N - H_{k+N}}{kN(k+N+1)N!}$$

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$$\sum_{k=1}^a \sum_{j=0}^{\infty} f(N, k, j) = \sum_{k=1}^a \frac{H_k + H_N - H_{k+N}}{kN(k+N+1)N!} \\ = \text{Sigma}$$

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$$\sum_{k=1}^{\infty} \sum_{j=0}^{\infty} f(N, k, j) = \sum_{k=1}^{\infty} \frac{H_k + H_N - H_{k+N}}{kN(k+N+1)N!} \\ = \frac{H_N^2 + H_N^{(2)}}{2N(N+1)!}$$

where

$$H_N^{(2)} = \sum_{i=1}^N \frac{1}{i^2}$$