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Colorado State University, Fort Collins, Colorado, USA

Minisymposium: Symbolic Combinatorics

Symbolic Summation for Combinatorial and Physical Problems

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You've Got Mail (7/2004)

From: Doron Zeilberger
To: Robin Pemantle, Herbert Wilf
CC:Carsten Schneider

Robin and Herb,

I am willing to bet that Carsten Schneider's SIGMA package
for handling sums with harmonic numbers (among others)
can do it in a jiffy. I am Cc-ing this to Carsten.

Carsten: please do it, and Cc- the answer to me.
-Doron

The problem

```
From: Robin Pemantle [University of Pennsylvania]
To: herb wilf; doron zeilberger

Herb, Doron,

I have a sum that, when I evaluate numerically, looks suspiciously
like it comes out to exactly 1.
Is there a way I can automatically decide this?
The sum may be written in many ways, but one is:
```

$$\sum_{n,k=1}^{\infty} \frac{S_1(k)(S_1(n+1)-1)}{kn(n+1)(k+n)}; \qquad S_1(k) := \sum_{i=1}^{k} \frac{1}{i} \; (= H_k).$$

[Arose in the analysis of the simplex algorithm on the Klee-Minty cube]

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

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

GIVEN

$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\, f(n,k)}.$$

Telescoping

GIVEN

$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\, f(n,k)}.$$

FIND $g(n,k)$:

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

for all $n, k \geq 1$.

Telescoping

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$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=: f(n,k)}.$$

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for all $n, k \geq 1$.

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

Telescoping

GIVEN

$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=: f(n,k)} .$$

FIND $g(n,k)$:

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for all $n, k \geq 1$.

no solution ☹

Zeilberger's creative telescoping paradigm

GIVEN

$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\,f(n,k)}.$$

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

$$\boxed{g(n,k+1)-g(n,k)} = \boxed{c_0(n)f(n,k)+c_1(n)\,f(n+1,k)}$$

for all $n,k \geq 1$.

no solution ☹

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$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\, f(n,k)}.$$

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

for all $n, k \geq 1$.

solution

Zeilberger's creative telescoping paradigm

GIVEN

$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\, f(n,k)}.$$

FIND $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

for all $n, k \geq 1$.

Sigma *computes*: $c_0(n) = n^2$, $c_1(n) = -(n+1)(2n+1)$, $c_2(n) = (n+1)(n+2)$

and

$$g(n,k) := -\frac{kS_1(k) + n + k}{(n+k)(n+k+1)},$$

$$g(n,k+1) := -\frac{(1+n)S_1(k) + n + k + 2}{(n+k+1)(n+k+2)}.$$

Zeilberger's creative telescoping paradigm

GIVEN

$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\, f(n,k)}.$$

FIND $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

for all $n,k\geq 1$.

Summing this equation over k from 1 to a gives:

$$\boxed{g(n,a+1)-g(n,1)} = \boxed{\sum_{k=1}^{a}\Big[c_0(n)f(n,k)+c_1(n)f(n+1,k)+c_2(n)f(n+2,k)\Big]}$$

Zeilberger's creative telescoping paradigm

GIVEN

$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\, f(n,k)} .$$

FIND $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

for all $n, k \geq 1$.

Summing this equation over k from 1 to a gives:

$$\boxed{g(n,a+1) - g(n,1)} = \boxed{\sum_{k=1}^{a} c_0(n) f(n,k) + \sum_{k=1}^{a} c_1(n) f(n+1,k) + \sum_{k=1}^{a} c_2(n) f(n+2,k)}$$

Zeilberger's creative telescoping paradigm

GIVEN

$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=: f(n,k)}.$$

FIND $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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for all $n, k \geq 1$.

Summing this equation over k from 1 to a gives:

$$\boxed{g(n,a+1) - g(n,1)} = \boxed{c_0(n)\sum_{k=1}^{a} f(n,k) + c_1(n)\sum_{k=1}^{a} f(n+1,k) + c_2(n)\sum_{k=1}^{a} f(n+2,k)}$$

Zeilberger's creative telescoping paradigm

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$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\, f(n,k)}.$$

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for all $n, k \geq 1$.

Summing this equation over k from 1 to a gives:

$$\boxed{g(n,a+1) - g(n,1)} = \boxed{c_0(n)\text{A'}(n) + c_1(n)\text{A'}(n+1) + c_2(n)\text{A'}(n+2)}$$

Zeilberger's creative telescoping paradigm

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$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\, f(n,k)}.$$

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for all $n, k \geq 1$.

Summing this equation over k from 1 to a gives:

$$\boxed{g(n,a+1) - g(n,1)} = \boxed{c_0(n)\text{A'}(n) + c_1(n)\text{A'}(n+1) + c_2(n)\text{A'}(n+2)}$$

$$||\qquad\qquad\qquad\qquad ||$$

$$\frac{a}{(n+1)(a+n+1)} - \frac{(a+1)S_1(a)}{(a+n+1)(a+n+2)} \qquad n^2\text{A'}(n) - (n+1)(2n+1)\text{A'}(n+1) + (n+1)(n+2)\text{A'}(n+2)$$

Summation principles (in difference field setting)

$$n^2\mathbf{A}(n) - (n+1)(2n+1)\mathbf{A}(n+1) + (n+1)(n+2)\mathbf{A}(n+2) = \frac{1}{n+1}$$

Recurrence finder

$$\mathbf{A}(n) = \sum_{k=1}^{\infty} \frac{S_1(k)}{k(k+n)}$$

Summation principles (in difference field setting)

$$n^2\mathbf{A}(n)-(n+1)(2n+1)\mathbf{A}(n+1)+(n+1)(n+2)\mathbf{A}(n+2)=\frac{1}{n+1}$$

Recurrence solver

$$\mathbf{A}(n)=\sum_{k=1}^{\infty}\frac{S_1(k)}{k(k+n)}\in\left\{c_1\frac{nS_1(n)-1}{n^2}+c_2\frac{1}{n}+\frac{nS_1(n)^2-2S_1(n)+nS_2(n)}{2n^2}\;\middle|\;c_1,c_2\in\mathbb{R}\right\}$$

where

$$S_2(n)=\sum_{i=1}^{n}\frac{1}{i^2}$$

Summation principles (in difference field setting)

$$n^2\mathbf{A}(n)-(n+1)(2n+1)\mathbf{A}(n+1)+(n+1)(n+2)\mathbf{A}(n+2)=\frac{1}{n+1}$$

Summation package Sigma

(based on difference field algorithms/theory
see, e.g., Karr 1981, Bronstein 2000, Schneider 2001 –)

$$\mathbf{A}(n)=\sum_{k=1}^{\infty}\frac{S_1(k)}{k(k+n)} = \boxed{0\frac{nS_1(n)-1}{n^2}+\zeta_2\frac{1}{n}+\frac{nS_1(n)^2-2S_1(n)+nS_2(n)}{2n^2}}$$

where

$$S_2(n)=\sum_{i=1}^{n}\frac{1}{i^2} \qquad \zeta_z=\sum_{i=1}^{\infty}\frac{1}{i^z}\ (=\zeta(z))$$

In[1]:= $<<$ **Sigma.m**

Sigma - A summation package by Carsten Schneider © RISC-Linz

In[2]:= $$\mathbf{mySum} = \sum_{k=1}^{a} \frac{S_1(k)}{k(k+n)}$$

In[1]:= << **Sigma.m**

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In[2]:= $$\mathbf{mySum} = \sum_{k=1}^{a} \frac{S_1(k)}{k(k+n)}$$

In[3]:= $\mathbf{rec = GenerateRecurrence[mySum, n][[1]]}$

Out[3]= $$n^2\mathrm{SUM}[n] - (n+1)(2n+1)\mathrm{SUM}[n+1] + (n+1)(n+2)\mathrm{SUM}[n+2] == \frac{(-a-1)S_1(a)}{(a+n+1)(a+n+2)} + \frac{a}{(n+1)(a+n+1)}$$

In[1]:= $<<$ **Sigma.m**

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In[4]:= **rec = LimitRec[rec, SUM[n], {n}, a]**

Out[4]= $$n^2\mathrm{SUM}[n] - (n+1)(2n+1)\mathrm{SUM}[n+1] + (n+1)(n+2)\mathrm{SUM}[n+2] = \frac{1}{n+1}$$

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In[4]:= $\mathbf{rec} = \mathbf{LimitRec[rec, SUM[n], \{n\}, a]}$

Out[4]= $n^2 \mathrm{SUM}[n] - (n+1)(2n+1)\mathrm{SUM}[n+1] + (n+1)(n+2)\mathrm{SUM}[n+2] = \frac{1}{n+1}$

In[5]:= $\mathbf{recSol} = \mathbf{SolveRecurrence[rec, SUM[n]]}$

Out[5]= $\left\{\left\{0, \frac{1}{n}\right\}, \left\{0, \frac{\sum_{i=1}^{n} \frac{1}{i}}{n} - \frac{1}{n^2}\right\}, \left\{1, \frac{\left(\sum_{i=1}^{n} \frac{1}{i}\right)^2}{2n} - \frac{\sum_{i=1}^{n} \frac{1}{i}}{n^2} + \frac{\sum_{i=1}^{n} \frac{1}{i^2}}{2n}\right\}\right\}$

In[1]:= << **Sigma.m**

Sigma - A summation package by Carsten Schneider © RISC-Linz

In[2]:= $\mathbf{mySum} = \sum_{k=1}^{a} \frac{S_1(k)}{k(k+n)}$

In[3]:= $\mathbf{rec = GenerateRecurrence[mySum, n][[1]]}$

Out[3]= $n^2 SUM[n] - (n+1)(2n+1)SUM[n+1] + (n+1)(n+2)SUM[n+2] == \frac{(-a-1)S_1(a)}{(a+n+1)(a+n+2)} + \frac{a}{(n+1)(a+n+1)}$

In[4]:= $\mathbf{rec = LimitRec[rec, SUM[n], \{n\}, a]}$

Out[4]= $n^2 SUM[n] - (n+1)(2n+1)SUM[n+1] + (n+1)(n+2)SUM[n+2] = \frac{1}{n+1}$

In[5]:= $\mathbf{recSol = SolveRecurrence[rec, SUM[n]]}$

Out[5]= $\{\{0, \frac{1}{n}\}, \{0, \frac{\sum_{i=1}^{n} \frac{1}{i}}{n} - \frac{1}{n^2}\}, \{1, \frac{(\sum_{i=1}^{n} \frac{1}{i})^2}{2n} - \frac{\sum_{i=1}^{n} \frac{1}{i}}{n^2} + \frac{\sum_{i=1}^{n} \frac{1}{i^2}}{2n}\}\}$

In[6]:= $\mathbf{FindLinearCombination[recSol, \{1, \{\zeta_2, 1/2 + \zeta_2/2\}\}, n, 2]}$

Out[6]= $-\frac{\sum_{i=1}^{n} \frac{1}{i}}{n^2} + \frac{(\sum_{i=1}^{n} \frac{1}{i})^2}{2n} + \frac{\sum_{i=1}^{n} \frac{1}{i^2}}{2n} + \frac{\zeta_2}{n}$

$$S=\sum_{n=1}^{\infty}\frac{S_1(n+1)-1}{n(n+1)}\qquad \underbrace{\boxed{\sum_{k=1}^{\infty}\frac{S_1(k)}{k(k+n)}}}_{\displaystyle =\frac{\zeta_2}{n}+\frac{nS_1(n)^2-2S_1(n)+nS_2(n)}{2n^2}}$$

$$S=\sum_{n=1}^{\infty}\frac{S_1(n+1)-1}{n(n+1)}\qquad \underbrace{\boxed{\sum_{k=1}^{\infty}\frac{S_1(k)}{k(k+n)}}}$$

$$=\frac{\zeta_2}{n}+\frac{nS_1(n)^2-2S_1(n)+nS_2(n)}{2n^2}$$

$$=-4\zeta_2+(\zeta_2-1)\sum_{i=1}^{\infty}\frac{S_1(i)}{i^2}-\sum_{i=1}^{\infty}\frac{S_1(i)^2}{i^3}$$

$$+\frac{1}{2}\sum_{i=1}^{\infty}\frac{S_1(i)^3}{i^2}+\frac{1}{2}\sum_{i=1}^{\infty}\frac{S_1(i)S_2(i)}{i^2}$$

$$S = \sum_{n=1}^{\infty} \frac{S_1(n+1)-1}{n(n+1)} \qquad \underbrace{\boxed{\sum_{k=1}^{\infty} \frac{S_1(k)}{k(k+n)}}}$$

$$= \frac{\zeta_2}{n} + \frac{nS_1(n)^2 - 2S_1(n) + nS_2(n)}{2n^2}$$

$$= -4\zeta_2 + (\zeta_2 - 1)\sum_{i=1}^{\infty}\frac{S_1(i)}{i^2} - \sum_{i=1}^{\infty}\frac{S_1(i)^2}{i^3}$$

$$+ \frac{1}{2}\sum_{i=1}^{\infty}\frac{S_1(i)^3}{i^2} + \frac{1}{2}\sum_{i=1}^{\infty}\frac{S_1(i)S_2(i)}{i^2}$$

$$= -4\zeta_2 - 2\zeta_3 + 4\zeta_2\zeta_3 + 2\zeta_5 = 0.999222...$$

J.M. Borwein and R. Girgensohn. Evaluation of triple Euler sums. *Electron. J. Combin.*, 3:1–27, 1996.
P. Flajolet and B. Salvy. Euler sums and contour integral representations. *Experim. Math.*, 7(1):15–35, 1998.

$$S = \sum_{n=1}^{\infty} \frac{S_1(n+1)-1}{n(n+1)} \qquad \underbrace{\boxed{\sum_{k=1}^{\infty} \frac{S_1(k)}{k(k+n)}}}$$

$$= \frac{\zeta_2}{n} + \frac{nS_1(n)^2 - 2S_1(n) + nS_2(n)}{2n^2}$$

$$= -4\zeta_2 + (\zeta_2 - 1)\sum_{i=1}^{\infty}\frac{S_1(i)}{i^2} - \sum_{i=1}^{\infty}\frac{S_1(i)^2}{i^3}$$

$$+ \frac{1}{2}\sum_{i=1}^{\infty}\frac{S_1(i)^3}{i^2} + \frac{1}{2}\sum_{i=1}^{\infty}\frac{S_1(i)S_2(i)}{i^2}$$

$$= -4\zeta_2 - 2\zeta_3 + 4\zeta_2\zeta_3 + 2\zeta_5 = 0.999222...$$

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J. Blümlein and D. J. Broadhurst and J. A. M. Vermaseren, The Multiple Zeta Value Data Mine, *Comput. Phys. Commun.*, 181:582–625, 2010.

Toolbox 1: Symbolic summation algorithms

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

GIVEN a definite sum

$$A(n)=\sum_{k=1}^{n} f(n,k);$$

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

FIND a recurrence for $A(n)$

Back to creative telescoping

Given

$$f(n,k)=\frac{S_1(k)}{k(k+n)};$$

Find $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

Back to creative telescoping

Given
$$f(n,k)=\frac{S_1(k)}{k(k+n)};$$
Find $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

A difference field for the **summand:**

Construct a rational function field

$$\mathbb{F}$$

and a field automorphism $\sigma:\mathbb{F}\to\mathbb{F}$ defined by

Back to creative telescoping

Given

$$f(n,k)=\frac{S_1(k)}{k(k+n)};$$

Find $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

A difference field for the **summand:**

Construct a rational function field

$$\mathbb{F}:=\mathbb{Q}(\mathbf{n})$$

and a field automorphism $\sigma:\mathbb{F}\to\mathbb{F}$ defined by

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

Back to creative telescoping

Given
$$f(n,k)=\frac{S_1(k)}{k(k+n)};$$
Find $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

A difference field for the **summand:**

Construct a rational function field

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

and a field automorphism $\sigma:\mathbb{F}\to\mathbb{F}$ defined by

$$\sigma(c)=c\quad\forall c\in\mathbb{Q}(n),$$
$$\sigma(\mathbf{k})=\mathbf{k}+\mathbf{1},\qquad\qquad \mathcal{S}\,k=k+1,$$

Back to creative telescoping

Given

$$f(n,k)=\frac{S_1(k)}{k(k+n)};$$

Find $g(n,k)$ and $c_0(n),c_1(n),c_2(n)$:

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

A difference field for the **summand:**

Construct a rational function field

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

$$\mathbb{F}:=\mathbb{Q}(n)(k)(\mathbf{s})$$

Karr 1981

and a field automorphism $\sigma:\mathbb{F}\to\mathbb{F}$ defined by

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

$$\sigma(k)=k+1,\qquad\qquad \mathcal{S}\,k=k+1,$$

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

Back to creative telescoping

Given

$$f(n,k) = \frac{S_1(k)}{k(+n)};$$

Find $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

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

$$\boxed{\sigma(g) - g} = \boxed{c_0\,\frac{s}{k(k+n)} + c_1\,\frac{s}{k(k+n+1)} + c_2\,\frac{s}{k(k+n+2)}}$$

Back to creative telescoping

Given

$$f(n,k) = \frac{S_1(k)}{k(+n)};$$

Find $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

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

$$\boxed{\sigma(g) - g} = \boxed{c_0 \frac{s}{k(k+n)} + c_1 \frac{s}{k(k+n+1)} + c_2 \frac{s}{k(k+n+2)}}$$

$$\downarrow$$

$$c_0 = n^2,\ c_1 = -(n+1)(2n+1),\ c_2 = (n+1)(n+2)$$

$$g = -\frac{ks+n+k}{(n+k)(n+k+1)}$$

Zeilberger's creative telescoping paradigm

GIVEN

$$\text{A'}(n) := \underbrace{\sum_{k=1}^{a} \frac{S_1(k)}{k(k+n)}}_{=: f(n,k)}.$$

FIND $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

for all $n, k \geq 1$.

Sigma *computes*: $c_0(n) = n^2$, $c_1(n) = -(n+1)(2n+1)$, $c_2(n) = (n+1)(n+2)$

and

$$g(n,k) := -\frac{kS_1(k) + n + k}{(n+k)(n+k+1)},$$

$$g(n,k+1) := -\frac{(1+n)S_1(k) + n + k + 2}{(n+k+1)(n+k+2)}.$$

Zeilberger's creative telescoping paradigm

GIVEN

$$\text{A'}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)}{k(k+n)}}_{=:\, f(n,k)}.$$

FIND $g(n,k)$ and $c_0(n), c_1(n), c_2(n)$:

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

for all $n, k \geq 1$.

Summing this equation over k from 1 to a gives:

$$\boxed{g(n,a+1) - g(n,1)} = \boxed{\sum_{k=1}^{a} \Big[c_0(n) f(n,k) + c_1(n) f(n+1,k) + c_2(n) f(n+2,k)\Big]}$$

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$$||\qquad\qquad\qquad ||$$

$$\frac{a}{(n+1)(a+n+1)} - \frac{(a+1)S_1(a)}{(a+n+1)(a+n+2)} \qquad n^2\text{A'}(n) - (n+1)(2n+1)\text{A'}(n+1) + (n+1)(n+2)\text{A'}(n+2)$$

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

GIVEN a definite sum

$$A(n) = \sum_{k=1}^{n} f(n,k);$$

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

FIND a recurrence for $A(n)$

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2. Recurrence solving

GIVEN a recurrence

$a_0(n), \dots, a_d(n), h(n)$:
indefinite nested product-sum expressions in n.

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

FIND all solutions expressible by indefinite nested products/sums in n.
(Abramov/Bronstein/Petkovšek/CS, in preparation)

Note: the sum solutions are highly nested
(possibly with denominators of high degrees)

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3. Simplify the solutions (using difference field theory) s.t.
   - the sums are algebraic independent
   - the sums can be given in terms of special functions

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4. Find a "closed form"

A(n)=combined solutions in terms of indefinite nested sums in n.

Iterative application from inside to outside transforms

definite multi-sums

$\downarrow$

indefinite nested sums

$$\sum_{j=0}^{n-2}\sum_{r=0}^{j+1}\sum_{s=0}^{n-j+s-2}\frac{(-1)^{r+s}\binom{j+1}{r}\binom{-j+n+r-2}{s}(-j+n-2)!r!}{(n-s)(s+1)(-j+n+r)!}$$

$$\sum_{j=0}^{n-2}\sum_{r=0}^{j+1}\sum_{s=0}^{n-j+s-2}\frac{(-1)^{r+s}\binom{j+1}{r}\binom{-j+n+r-2}{s}(-j+n-2)!r!}{(n-s)(s+1)(-j+n+r)!}$$

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$$||$$

$$\boxed{\binom{j+1}{r}\Big(\frac{(-1)^{r}(-j+n-2)!r!}{(n+1)(-j+n+r-1)(-j+n+r)!}+\frac{(-1)^{n+r}(j+1)!(-j+n-2)!(-j+n-1)_r r!}{(n-1)n(n+1)(-j+n+r)!(-j-1)_r(2-n)_j}\Big)}$$

$$\sum_{j=0}^{n-2}\sum_{r=0}^{j+1}\sum_{s=0}^{n-j+s-2}\frac{(-1)^{r+s}\binom{j+1}{r}\binom{-j+n+r-2}{s}(-j+n-2)!r!}{(n-s)(s+1)(-j+n+r)!}$$

$$\|$$

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$$||$$

$$\boxed{\Big(\frac{n^2-n+1}{(n-1)^2n^2(n+1)(2-n)_j}+\frac{\sum_{i=1}^{j}\frac{(2-n)_i}{(-i+n-1)^2(i+1)!}}{(n+1)(2-n)_j}+\frac{(-1)^{j+n}(-j-2)(-j+n-2)!}{(j-n+1)(n+1)^2n!}\Big)(j+1)!-\frac{1}{(n+1)^2(-j+n-1)}}$$

$$\sum_{j=0}^{n-2}\sum_{r=0}^{j+1}\sum_{s=0}^{n-j+s-2}\frac{(-1)^{r+s}\binom{j+1}{r}\binom{-j+n+r-2}{s}(-j+n-2)!r!}{(n-s)(s+1)(-j+n+r)!}$$

$$||$$

$$\sum_{j=0}^{n-2}\Bigg(\Big(\frac{n^2-n+1}{(n-1)^2n^2(n+1)(2-n)_j}+\frac{\sum_{i=1}^{j}\frac{(2-n)_i}{(-i+n-1)^2(i+1)!}}{(n+1)(2-n)_j}+$$
$$\frac{(-1)^{j+n}(-j-2)(-j+n-2)!}{(j-n+1)(n+1)^2n!}\Big)(j+1)!-\frac{1}{(n+1)^2(-j+n-1)}\Bigg)$$

$$\sum_{j=0}^{n-2}\sum_{r=0}^{j+1}\sum_{s=0}^{n-j+s-2}\frac{(-1)^{r+s}\binom{j+1}{r}\binom{-j+n+r-2}{s}(-j+n-2)!r!}{(n-s)(s+1)(-j+n+r)!}$$

$$||$$

$$\sum_{j=0}^{n-2}\left(\left(\frac{n^2-n+1}{(n-1)^2n^2(n+1)(2-n)_j}+\frac{\sum_{i=1}^{j}\frac{(2-n)_i}{(-i+n-1)^2(i+1)!}}{(n+1)(2-n)_j}+\frac{(-1)^{j+n}(-j-2)(-j+n-2)!}{(j-n+1)(n+1)^2n!}\right)(j+1)!-\frac{1}{(n+1)^2(-j+n-1)}\right)$$

$$||$$

$$\frac{-n^2-n-1}{n^2(n+1)^3}+\frac{(-1)^n\left(n^2+n+1\right)}{n^2(n+1)^3}-\frac{2S_{-2}(n)}{n+1}+\frac{S_1(n)}{(n+1)^2}+\frac{S_2(n)}{-n-1}$$

Note: $S_a(n)=\sum_{i=1}^{n}\frac{\mathsf{sign}(a)^i}{i^{|a|}},\ a\in\mathbb{Z}\setminus\{0\}.$

Toolbox 2: Special function algorithms

Computer algebra and special functions:

Harmonic sums (Borwein, Vermaseren, Remmiddi, Blümlein; Hoffman, Broadhurst,...)

$$S_{2,1}(n) = \boxed{\sum_{i=1}^{n} \frac{1}{i^2} \sum_{j=1}^{i} \frac{1}{j}}$$

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Integral representation:

$$= \int_0^1 \frac{x^n - 1}{1 - x} \left(\int_0^x \frac{\int_0^y \frac{1}{1-z} dz}{y} dy - \zeta_2 \right) dx, \qquad \zeta_z := \sum_{i=1}^{\infty} 1/i^z$$

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Asymptotic expansion:

$$= \left(\frac{1}{30n^5} - \frac{1}{6n^3} + \frac{1}{2n^2} - \frac{1}{n} \right) \ln(n)$$
$$- \frac{1}{100n^5} - \frac{1}{6n^4} + \frac{13}{36n^3} - \frac{1}{4n^2} - \frac{1}{n} + 2\zeta_3 + O\left(\frac{\ln(n)}{n^6}\right).$$

limit computations **numerical evaluation**

Computer algebra and special functions:

Generalization to cyclotomic harmonic sums

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

Integral representation:

$$=-(-1)^n\int_0^1\frac{x^{2n}}{x^2+1}dx+\frac{(-1)^n}{2n+1}-1+\frac{\pi}{4},$$

Asymptotic expansion:

$$=(-1)^n\left(-\tfrac{3}{64n^5}-\tfrac{1}{16n^4}+\tfrac{3}{16n^3}-\tfrac{1}{4n^2}+\tfrac{1}{4n}\right)+\tfrac{\pi}{4}-1+O(\tfrac{1}{n^6})$$

limit computations **numerical evaluation**

(J. Ablinger, J. Blümlein, CS; J. Math. Phys. 2011 [arXiv:1105.6063 [math-ph]])

The full machinery:

In[1]:= $<<$ **Sigma.m**

Sigma by Carsten Schneider © RISC-Linz

In[2]:= $<<$ **EvaluateMultiSums.m**

EvaluateMultiSums by Carsten Schneider © RISC-Linz

In[4]:= $$\mathbf{EvaluateMultiSum}\Big[\sum_{n=1}^{\infty}\sum_{k=1}^{\infty}\frac{S[1,k](S[1,n+1]-1)}{kn(n+1)(k+n)}\Big]$$

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Out[4]= $$3\sum_{i=1}^{\infty}\frac{\sum_{j=1}^{i}\frac{\sum_{k=1}^{j}\frac{\sum_{l=1}^{k}\frac{1}{l}}{k}}{j}}{i^2}-2\sum_{j=1}^{\infty}\frac{\sum_{k=1}^{j}\frac{\sum_{l=1}^{k}\frac{1}{l}}{k}}{j^3}+\frac{1}{3}\Big(3\sum_{j=1}^{\infty}\frac{\sum_{k=1}^{j}\frac{\sum_{l=1}^{k}\frac{1}{l}}{k^2}}{j^2}-3\sum_{k=1}^{\infty}\frac{\sum_{l=1}^{k}\frac{1}{l}}{k^4}\Big)-$$
$$2\sum_{k=1}^{\infty}\frac{\sum_{l=1}^{k}\frac{1}{l^3}}{k^2}+\Big(\sum_{l=1}^{\infty}\frac{1}{l^2}\Big)\Big(-\sum_{k=1}^{\infty}\frac{\sum_{l=1}^{k}\frac{1}{l}}{k^2}+\sum_{l=1}^{\infty}\frac{1}{l^3}-1\Big)+z_2\Big(\sum_{k=1}^{\infty}\frac{\sum_{l=1}^{k}\frac{1}{l}}{k^2}-1\Big)+\sum_{l=1}^{\infty}\frac{1}{l^5}$$

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Out[5]= $-10\zeta_3 + \zeta_2^2\left(\frac{58\zeta_3}{5} - \frac{29}{5}\right) - 10\zeta_5 + \zeta_2(-\zeta_3 + 13\zeta_5 - 4) + \frac{457\zeta_7}{8}$

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Out[5]= $2\zeta_3+\zeta_2^2\left(\frac{17\zeta_3}{10}+\frac{17}{10}\right)+\zeta_2(2\zeta_3-3\zeta_5-4)-\frac{9\zeta_5}{2}+\frac{3\zeta_7}{16}$

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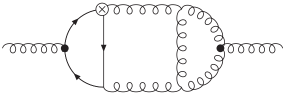
Out[5]= $3\zeta_3^2 - \frac{15\zeta_5}{2} + \zeta_2(9\zeta_5 - 6\zeta_3) + \frac{149\zeta_7}{16} + \frac{114}{35}\zeta_2^3$

Evaluation of Feynman diagrams

(long term project with J. Blümlein, Deutsches Elektronen–Synchrotron)



Behavior of particles

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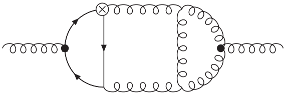


Behavior of particles

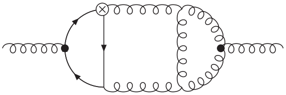
$$\longrightarrow$$

$$\int \Phi(n, \epsilon, x)dx$$

Feynman integrals

Evaluation of Feynman diagrams

(long term project with J. Blümlein, Deutsches Elektronen–Synchrotron)



Behavior of particles

$$\int \Phi(n,\epsilon,x)dx$$

Feynman integrals

DESY

$$\sum f(n,\epsilon,k)$$

multi sums

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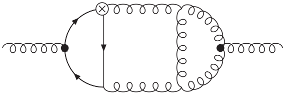

Behavior of particles → $\int \Phi(n, \epsilon, x)dx$

Feynman integrals

↓ **DESY**

$\sum f(n, \epsilon, k)$

multi sums

symbolic summation

simple sum expressions ←

Evaluation of Feynman diagrams

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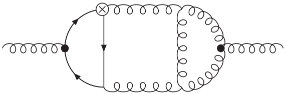

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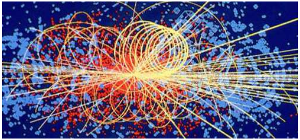


Evaluations required for the LHC experiment at CERN

DESY

$$\sum f(n,\epsilon,k)$$

multi sums

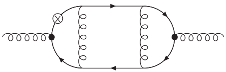
symbolic summation

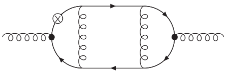
simple sum expressions

processable by physicists

Example: 3–Loop Ladder Graphs

Joint work with J. Ablinger (RISC), J. Blümlein (DESY), A. Hasselhuhn (DESY), S. Klein (RWTH), F. Wissbrock (DESY)

 (massive 3–loop ladder graph with operator insertion)

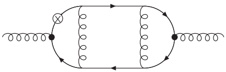


J. Blümlein
A. Hasselhuhn

$$= \frac{C_3}{(n+1)(n+2)} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{l=2}^{n+2} \binom{n+2}{l} \sum_{j=2}^{l} \binom{l}{j} \Bigg\{$$

$$\sum_{k=1}^{j} \binom{j}{k} \sum_{r=0}^{l-k} \binom{l-k}{r} (-1)^{l+j+k+r} \frac{B\left(k, m+1+\frac{\varepsilon}{2}\right)\Gamma(k+r+m+n+\frac{\varepsilon}{2})}{\Gamma(m+1)\Gamma(n+1)\Gamma(k+r+\frac{\varepsilon}{2})} \frac{B\left(r+l-1, n+1+\frac{\varepsilon}{2}\right)}{(n+3-j)} \frac{B\left(k+m-\frac{\varepsilon}{2}, r+1+n-\cdots\right.}{(k+r+1+m+n-\varepsilon\cdots}$$

$$+ \sum_{r=0}^{l-j} \binom{l-j}{r} (-1)^{l+j+r} \frac{B\left(r+l-1, n+1+\frac{\varepsilon}{2}\right)\Gamma(j+r+m+n+\frac{\varepsilon}{2})}{\Gamma(m+1)\Gamma(n+1)\Gamma(j+r+\frac{\varepsilon}{2})} \frac{B\left(j, m+1+\frac{\varepsilon}{2}\right) B\left(j+m-\frac{\varepsilon}{2}, r+1+n-\frac{\varepsilon}{2}\right)}{(j+r+1+m+n-\varepsilon)(n+3-j)} \Bigg\}$$



J. Blümlein
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|| EvaluateMultiSums

$$\frac{C_3}{(n+1)(n+2)(n+3)} \Bigg\{ \tfrac{1}{6} S_1^3(n) + \tfrac{n^2+12n+16}{2(n+1)(n+2)} S_1(n)^2 + \tfrac{4(2n+3)}{(n+1)^2(n+2)} S_1(n)$$

$$+ 2\left[-2^{n+3} + 3 - (-1)^n\right]\zeta_3 + \left[\tfrac{3n^2+40n+56}{2(n+1)(n+2)} - \tfrac{1}{2} S_1(n)\right] S_2(n)$$

$$- (-1)^n S_{-3}(n) + \tfrac{8(2n+3)}{(n+1)^3(n+2)} - \tfrac{3n+17}{3} S_3(n) - 2(-1)^n S_{-2,1}(n) - (n+3) S_{2,1}(n)$$

$$+ 2^{n+4} S_{1,2}\left(\frac{1}{2},1;n\right) + 2^{n+3} \boxed{S_{1,1,1}\left(\frac{1}{2},1,1;n\right)} \Bigg\} + O(\varepsilon)$$

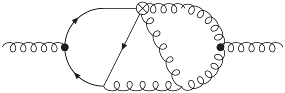
$$\boxed{S_{1,1,1}\left(\frac{1}{2},1,1;n\right)} = \sum_{i=1}^{n} \frac{\left(\frac{1}{2}\right)^{i} \sum_{j=1}^{i} \frac{\sum_{k=1}^{j} \frac{1}{k}}{j}}{i}$$

$$\boxed{S_{1,1,1}\left(\frac{1}{2},1,1;n\right)} = \sum_{i=1}^{n} \frac{\left(\frac{1}{2}\right)^i \sum_{j=1}^{i} \frac{\sum_{k=1}^{j} \frac{1}{k}}{j}}{i}$$

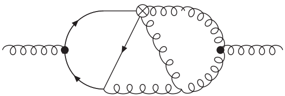
|| asymptotic expansion (HarmonicSums package)

$$2^{-n}\left(+\frac{541}{n^6}-\frac{75}{n^5}+\frac{13}{n^4}-\frac{3}{n^3}+\frac{1}{n^2}-\frac{1}{2n}\right)(\ln(n)+\gamma)^2$$
$$+2^{-n-3}\left(-\frac{114686}{5n^6}+\frac{44099}{15n^5}-\frac{1372}{3n^4}+\frac{266}{3n^3}-\frac{20}{n^2}\right)(\ln(n)+\gamma)$$
$$+2^{-n}\left(+\frac{541}{n^6}-\frac{75}{n^5}+\frac{13}{n^4}-\frac{3}{n^3}+\frac{1}{n^2}-\frac{1}{2n}\right)\zeta_2+\frac{3\zeta_3}{4}$$
$$+2^{-n-9}\left(\frac{69280576}{45n^6}-\frac{1582096}{9n^5}+\frac{69184}{3n^4}-\frac{3264}{n^3}+\frac{256}{n^2}\right)+O\left(\frac{1}{2^n n^7}\right)$$

(J. Ablinger, J. Blümlein, CS; arXiv:1302.0378 [math-ph])



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



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

Simplify

$$||$$

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

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

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

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

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

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

$$\frac{7}{12}S_1(n)^4+\frac{(17n+5)S_1(n)^3}{3n(n+1)}+\Big(\frac{35n^2-2n-5}{2n^2(n+1)^2}+\frac{13S_2(n)}{2}+\frac{5(-1)^n}{2n^2}\Big)S_1(n)^2$$
$$+\Big(-\frac{4(13n+5)}{n^2(n+1)^2}+\Big(\frac{4(-1)^n(2n+1)}{n(n+1)}-\frac{13}{n}\Big)S_2(n)+\Big(\frac{29}{3}-(-1)^n\Big)S_3(n)$$
$$+\big(2+2(-1)^n\big)S_{2,1}(n)-28S_{-2,1}(n)+\frac{20(-1)^n}{n^2(n+1)}\Big)S_1(n)+\Big(\frac{3}{4}+(-1)^n\Big)S_2(n)^2$$
$$-2(-1)^nS_{-2}(n)^2+S_{-3}(n)\Big(\frac{2(3n-5)}{n(n+1)}+\big(26+4(-1)^n\big)S_1(n)+\frac{4(-1)^n}{n+1}\Big)$$
$$+\Big(\frac{(-1)^n(5-3n)}{2n^2(n+1)}-\frac{5}{2n^2}\Big)S_2(n)+S_{-2}(n)\Big(10S_1(n)^2+\Big(\frac{8(-1)^n(2n+1)}{n(n+1)}$$
$$+\frac{4(3n-1)}{n(n+1)}\Big)S_1(n)+\frac{8(-1)^n(3n+1)}{n(n+1)^2}+\big(-22+6(-1)^n\big)S_2(n)-\frac{16}{n(n+1)}\Big)$$
$$+\Big(\frac{(-1)^n(9n+5)}{n(n+1)}-\frac{29}{3n}\Big)S_3(n)+\Big(\frac{19}{2}-2(-1)^n\Big)S_4(n)+\big(-6+5(-1)^n\big)S_{-4}(n)$$
$$+\Big(-\frac{2(-1)^n(9n+5)}{n(n+1)}-\frac{2}{n}\Big)S_{2,1}(n)+\big(20+2(-1)^n\big)S_{2,-2}(n)+\big(-17+13(-1)^n\big)S_{3,1}(n)$$
$$-\frac{8(-1)^n(2n+1)+4(9n+1)}{n(n+1)}S_{-2,1}(n)-\big(24+4(-1)^n\big)S_{-3,1}(n)+\big(3-5(-1)^n\big)S_{2,1,1}(n)$$
$$+32S_{-2,1,1}(n)+\left(\frac{3}{2}S_1(n)^2-\frac{3S_1(n)}{n}+\frac{3}{2}(-1)^nS_{-2}(n)\right)\zeta_2$$

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For further details see
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  See this talk

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- **Computer Algebra for Nested Sums and Products** (CS)
  See this talk
- **Computer Algebra and Combinatorial Inequalities** (V. Pillwein)
  The aim here is to develop new methods for proving combinatorial inequalities using a combination of symbolic algorithms and classical techniques from enumerative combinatorics.

For further details see
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