Toronto, Fields Institute, December 15, 2015

Workshop on Algebra, Geometry and Proofs in Symbolic Computation

Symbolic summation for particle physics: difference ring theory, stable software and proof certificates

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Der Wissenschaftsfonds

Some of the available summation tools:

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Koornwinder, T.H.: On Zeilberger's algorithm and its q-analogue. J. Comp. Appl. Math. **48**, 91–111 (1993)

Koutschan, C.: Creative telescoping for holonomic functions. In: C. Schneider, J. Blümlein (eds.) Computer Algebra in Quantum Field Theory: Integration, Summation and Special Functions, Texts and Monographs in Symbolic Computation, pp. 171–194. Springer (2013). ArXiv:1307.4554 [cs.SC]

Paule, P.: Greatest factorial factorization and symbolic summation. J. Symbolic Comput. **20**(3), 235–268 (1995)

Paule, P.: Contiguous relations and creative telescoping. unpublished manuscript p. 33 pages (2001)

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Petkovšek, M.: Hypergeometric solutions of linear recurrences with polynomial coefficients. J. Symbolic Comput. **14**(2-3), 243–264 (1992)

Petkovšek, M., Wilf, H.S., Zeilberger, D.: $A = B$. A. K. Peters, Wellesley, MA (1996)

Petkovšek, M., Zakrajšek, H.: Solving linear recurrence equations with polynomial coefficients. In: C. Schneider, J. Blümlein (eds.) Computer Algebra in Quantum Field Theory: Integration, Summation and Special Functions, Texts and Monographs in Symbolic Computation, pp. 259–284. Springer (2013)

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Zeilberger, D., 1990. A holonomic systems approach to special functions identities. J. Comput. Appl. Math. 32, 321–368.

Zeilberger, D.: The method of creative telescoping. J. Symbolic Comput. **11**, 195–204 (1991)

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Here I will restrict to the setting of difference rings/fields.

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}(\underbrace{\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}}_{f(j)})$$

where

$$S_1(n) = \sum_{i=1}^{n}\frac{1}{i} \quad (= H_n)$$

Arose in the context of

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

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\underbrace{\Big(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}}_{f(j)}\Big)$$

FIND $g(j)$:

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

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Big(\underbrace{\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}}_{f(j)}\Big)$$

FIND $g(j)$:

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

$\uparrow$ summation package Sigma

$$g(j)=\frac{(j+k+1)(j+n+1)j!k!(j+k+n)!\Big(S_1(j)-S_1(j+k)-S_1(j+n)+S_1(j+k+n)\Big)}{kn(j+k+1)!(j+n+1)!(k+n+1)!}$$

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Big(\underbrace{\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}}_{f(j)}\Big)$$

FIND $g(j)$:

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

Summing the telescoping equation over j from 0 to a gives

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

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}(\underbrace{\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}}_{f(j)})$$

FIND $g(j)$:

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Summing the telescoping equation over j from 0 to a gives

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

$$= \underbrace{\frac{(a+1)!(k-1)!(a+k+n+1)!(S_1(a)-S_1(a+k)-S_1(a+n)+S_1(a+k+n))}{n(a+k+1)!(a+n+1)!(k+n+1)!} + \frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)n!} + \frac{(2a+k+n+2)a!k!(a+k+n)!}{(a+k+1)(a+n+1)(a+k+1)!(a+n+1)!(k+n+1)!}}_{a\to\infty}$$

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Big(\underbrace{\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}}_{f(j)}\Big)$$

$$\sum_{j=0}^{\infty} f(j) = \qquad \frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)}$$

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\underbrace{\Big(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}\Big)}_{f(j)}$$

$$\sum_{k=1}^{\infty}\sum_{j=0}^{\infty}f(j)=\frac{1}{n!}\sum_{k=1}^{\infty}\frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)}$$

Telescoping

GIVEN

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

FIND $g(k)$:

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

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

no solution ☹

Zeilberger's creative telescoping paradigm

GIVEN

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

FIND $g(n,k)$

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

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

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

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

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

Sigma *computes*: $c_0(n) = -n$, $c_1(n) = (n+2)$ and

$$g(n,k) = \frac{kS_1(k)+(-n-1)S_1(n)-kS_1(k+n)-2}{(k+n+1)(n+1)^2}$$

Zeilberger's creative telescoping paradigm

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

Summing this equation over k from 1 to a gives:

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

Zeilberger's creative telescoping paradigm

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Zeilberger's creative telescoping paradigm

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Zeilberger's creative telescoping paradigm

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for all $0 \le k \le n$ and all $n \ge 0$.

Summing this equation over k from 1 to a gives:

$$\boxed{g(n,a+1)-g(n,1)} = \boxed{c_0(n)\,\mathsf{A}(n) + c_1(n)\,\mathsf{A}(n+1)}$$

Zeilberger's creative telescoping paradigm

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

$$\frac{(a+1)(S_1(a)+S_1(n)-S_1(a+n))}{(n+1)^2(a+n+2)} + \frac{a(a+1)}{(n+1)^3(a+n+1)(a+n+2)} \qquad -n\mathsf{A}(n)+(2+n)\mathsf{A}(n+1)$$

$$(n+2)\mathbf{A}(n+1) - n\mathbf{A}(n) = \frac{(n+1)S_1(n)+1}{(n+1)^3}$$

recurrence finder

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

$$(n+2)\mathbf{A}(n+1) - n\mathbf{A}(n) = \frac{(n+1)S_1(n)+1}{(n+1)^3}$$

recurrence solver

$$\boxed{A(n) = \sum_{k=1}^{\infty} \frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)}} \in \boxed{\{c \times \frac{1}{n(n+1)} + \frac{S_1(n)^2+S_2(n)}{2n(n+1)} | c \in \mathbb{R}\}}$$

where

$$S_1(n) = \sum_{i=1}^{n} \frac{1}{i} \qquad S_2(n) = \sum_{i=1}^{n} \frac{1}{i^2}$$

$$(n+2)\mathbf{A}(n+1) - n\mathbf{A}(n) = \frac{(n+1)S_1(n)+1}{(n+1)^3}$$

Summation package Sigma

(based on difference field/ring algorithms/theory
see, e.g., Karr 1981, Bronstein 2000, Schneider 2001/2004/2005a–c/2007/2008/2010a–c)

$$\boxed{A(n) = \sum_{k=1}^{\infty} \frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)}} = \boxed{0 \times \frac{1}{n(n+1)} + \frac{S_1(n)^2+S_2(n)}{2n(n+1)}}$$

where

$$S_1(n) = \sum_{i=1}^{n} \frac{1}{i} \qquad S_2(n) = \sum_{i=1}^{n} \frac{1}{i^2}$$

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\underbrace{\Big(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\left(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n)\right)}{(j+k+1)!(j+n+1)!(k+n+1)!}\Big)}_{f(j)}$$

$$\sum_{k=1}^{\infty}\sum_{j=0}^{\infty} f(j) = \frac{1}{n!}\sum_{k=1}^{\infty}\frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)}$$

$$= \frac{1}{n!}\frac{S_1(n)^2+S_2(n)}{2n(n+1)}$$

where

$$S_1(n)=\sum_{i=1}^{n}\frac{1}{i} \qquad S_2(n)=\sum_{i=1}^{n}\frac{1}{i^2}$$

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\underbrace{\Big(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}\Big)}_{f(n,k,j)}$$

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f(n,k,j) = \frac{S_1(n)^2+3S_2(n)}{2n(n+1)!}$$

where

$$S_1(n)=\sum_{i=1}^{n}\frac{1}{i} \qquad S_2(n)=\sum_{i=1}^{n}\frac{1}{i^2}$$

Toolbox 1: Indefinite summation

Toolbox 2: Definite summation

Toolbox 3: Special function algorithms

Toolbox 1: Indefinite summation

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 $n \geq 0$.

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 $n \geq 0$.

Sigma compute

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

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 $n \geq 0$.

Summing this equation over k from 1 to n gives

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

Telescoping in the given difference ring

FIND a closed form for

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

A difference ring for the summand

Consider a ring

$$\mathbb{A}$$

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

Telescoping in the given difference ring

FIND a closed form for
$$\sum_{k=1}^{n} S_1(k).$$

A difference ring for the summand

Consider a ring
$$\mathbb{A} := \mathbb{Q}$$

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

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

Telescoping in the given difference ring

FIND a closed form for

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

A difference ring for the summand

Consider a ring

$$\mathbb{A} := \mathbb{Q}(k)$$

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

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

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

Telescoping in the given difference ring

FIND a closed form for

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

A difference ring for the summand

Consider a ring

$$\mathbb{A} := \mathbb{Q}(k)[h]$$

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

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

Telescoping in the given difference ring

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

$$\boxed{\sigma(g) - g = h.}$$

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

with

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

Hence,

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

Toolbox 1: Indefinite summation – the basic tactic

(inspired by Karr's algorithm, 1981)

CONSTRUCT a difference ring $(\mathbb{A}, \sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}}$$

- with an automorphism where $\sigma(c) = c$ for all $c \in \mathbb{K}$ and where

CONSTRUCT a difference ring $(\mathbb{A}, \sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)}$$

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

CONSTRUCT a difference ring $(\mathbb{A}, \sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)}$$

- with an automorphism where $\sigma(c) = c$ for all $c \in \mathbb{K}$ and where

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

Sk!=(k+1)k! $\quad\leftrightarrow\quad$ $\sigma(p_1) = (k+1)p_1$

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hypergeometric expression $\leftrightarrow$ $\sigma(p_1) = a_1\, p_1 \qquad a_1 \in \mathbb{K}(k)^*$

CONSTRUCT a difference ring $(\mathbb{A}, \sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)(p_2)}$$

- with an automorphism where $\sigma(c) = c$ for all $c \in \mathbb{K}$ and where

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

$$\begin{array}{rcll} \text{hypergeometric} & \leftrightarrow & \sigma(p_1) = a_1\, p_1 & a_1 \in \mathbb{K}(k)^* \\ \text{expression} & & \sigma(p_2) = a_2 p_2 & a_2 \in \mathbb{K}(k)(p_1)^* \end{array}$$

CONSTRUCT a difference ring $(\mathbb{A}, \sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)(p_2)\dots(p_e)}$$

- with an automorphism where $\sigma(c) = c$ for all $c \in \mathbb{K}$ and where

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

hypergeometric expression $\leftrightarrow$

$$\begin{array}{ll} \sigma(p_1) = a_1\, p_1 & a_1 \in \mathbb{K}(k)^* \\ \sigma(p_2) = a_2 p_2 & a_2 \in \mathbb{K}(k)(p_1)^* \\ \vdots & \\ \sigma(p_e) = a_e p_e & a_e \in \mathbb{K}(k)(p_1, \dots, p_{e-1})^* \end{array}$$

CONSTRUCT a difference ring $(\mathbb{A}, \sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)(p_2)\dots(p_e)[x]}$$

- with an automorphism where $\sigma(c) = c$ for all $c \in \mathbb{K}$ and where

$$\begin{array}{rccl}
 & & \sigma(k) = k + 1 & \\
\text{hypergeometric} & \leftrightarrow & \sigma(p_1) = a_1\, p_1 & a_1 \in \mathbb{K}(k)^* \\
\text{expression} & & \sigma(p_2) = a_2 p_2 & a_2 \in \mathbb{K}(k)(p_1)^* \\
 & & \vdots & \\
 & & \sigma(p_e) = a_e p_e & a_e \in \mathbb{K}(k)(p_1, \dots, p_{e-1})^* \\
(-\mathbf{1})^{\mathbf{k}} & \leftrightarrow & \sigma(\mathbf{x}) = -\mathbf{x} & \mathbf{x}^{\mathbf{2}} = \mathbf{1}
\end{array}$$

CONSTRUCT a difference ring $(\mathbb{A}, \sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)(p_2)\dots(p_e)[x][s_1]}$$

- with an automorphism where $\sigma(c) = c$ for all $c \in \mathbb{K}$ and where

$$\begin{array}{rcll} & & \sigma(k) = k + 1 & \\ \text{hypergeometric} & \leftrightarrow & \sigma(p_1) = a_1\,p_1 & a_1 \in \mathbb{K}(k)^* \\ \text{expression} & & \sigma(p_2) = a_2 p_2 & a_2 \in \mathbb{K}(k)(p_1)^* \\ & & \vdots & \\ & & \sigma(p_e) = a_e p_e & a_e \in \mathbb{K}(k)(p_1, \dots, p_{e-1})^* \\ (-\mathbf{1})^{\mathbf{k}} & \leftrightarrow & \sigma(\mathbf{x}) = -\mathbf{x} & \mathbf{x}^{\mathbf{2}} = \mathbf{1} \\ \mathcal{S}S_1(k) = S_1(k) + \frac{1}{k+1} & \leftrightarrow & \sigma(s_1) = s_1 + \frac{1}{k+1} & \end{array}$$

CONSTRUCT a difference ring $(\mathbb{A}, \sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)(p_2)\dots(p_e)[x][s_1]}$$

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\text{hypergeometric} & \leftrightarrow & \sigma(p_1) = a_1\,p_1 & a_1 \in \mathbb{K}(k)^* \\
\text{expression} & & \sigma(p_2) = a_2 p_2 & a_2 \in \mathbb{K}(k)(p_1)^* \\
 & & \vdots & \\
 & & \sigma(p_e) = a_e p_e & a_e \in \mathbb{K}(k)(p_1,\dots,p_{e-1})^* \\
\mathbf{(-1)^k} & \leftrightarrow & \boldsymbol{\sigma(\mathbf{x}) = -\mathbf{x}} & \mathbf{x^2 = 1} \\
\text{sum} & \leftrightarrow & \sigma(s_1) = s_1 + f_1 & f_1 \in \mathbb{K}(k)(p_1,\dots,p_e)[x]
\end{array}
$$

CONSTRUCT a difference ring $(\mathbb{A}, \sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)(p_2)\dots(p_e)[x][s_1][s_2]}$$

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\end{array}$$

CONSTRUCT a difference ring $(\mathbb{A},\sigma)$:

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)(p_2)\dots(p_e)[x][s_1][s_2][s_3]\dots}$$

- with an automorphism where $\sigma(c)=c$ for all $c\in\mathbb{K}$ and where

$$\begin{array}{rclcl}
 & & \sigma(k)=k+1 & & \\
\text{hypergeometric} & \leftrightarrow & \sigma(p_1)=a_1\,p_1 & & a_1\in\mathbb{K}(k)^* \\
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 & & \vdots & & \\
 & & \sigma(p_e)=a_ep_e & & a_e\in\mathbb{K}(k)(p_1,\dots,p_{e-1})^* \\
\mathbf{(-1)^k} & \leftrightarrow & \boldsymbol{\sigma(\mathbf{x})=-\mathbf{x}} & & \mathbf{x^2=1} \\
\text{sum} & \leftrightarrow & \sigma(s_1)=s_1+f_1 & & f_1\in\mathbb{K}(k)(p_1,\dots,p_e)[x] \\
 & & \sigma(s_2)=s_2+f_2 & & f_2\in\mathbb{K}(k)(p_1,\dots,p_e)[x][s_1] \\
 & & \sigma(s_3)=s_3+f_3 & & f_3\in\mathbb{K}(k)(p_1,\dots,p_e)[x][s_1][s_2] \\
 & & \vdots & &
\end{array}$$

CONSTRUCT a $R\Pi\Sigma^*$-ring $(\mathbb{A},\sigma)$: (Karr81,CS14,CS15)

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)(p_2)\dots(p_e)[x][s_1][s_2][s_3]\dots}$$

- with an automorphism where $\sigma(c)=c$ for all $c\in\mathbb{K}$ and where

$$
\begin{array}{rclll}
 & & \sigma(k) = k+1 & \\
\text{hypergeometric} & \leftrightarrow & \sigma(p_1) = a_1\,p_1 & a_1 \in \mathbb{K}(k)^* \\
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 & & \sigma(s_2) = s_2+f_2 & f_2 \in \mathbb{K}(k)(p_1,\dots,p_e)[x][s_1] \\
 & & \sigma(s_3) = s_3+f_3 & f_3 \in \mathbb{K}(k)(p_1,\dots,p_e)[x][s_1][s_2] \\
 & & \vdots &
\end{array}
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such that $\mathrm{const}_\sigma\mathbb{A} = \{c\in\mathbb{A}|\sigma(c)=c\} = \mathbb{K}$.

CONSTRUCT a $R\Pi\Sigma^*$-ring $(\mathbb{A},\sigma)$: (Karr81,CS14,CS15)

- a ring (containing $\mathbb{Q}$)

$$\boxed{\mathbb{A} := \mathbb{K}(k)(p_1)(p_2)\dots(p_e)[x][s_1][s_2][s_3]\dots}$$

- with an automorphism where $\sigma(c)=c$ for all $c\in\mathbb{K}$ and where

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

hypergeometric expression $\leftrightarrow$

$$\begin{aligned}
\sigma(p_1) &= a_1\,p_1 && a_1\in\mathbb{K}(k)^*\\
\sigma(p_2) &= a_2 p_2 && a_2\in\mathbb{K}(k)(p_1)^*\\
&\vdots\\
\sigma(p_e) &= a_e p_e && a_e\in\mathbb{K}(k)(p_1,\dots,p_{e-1})^*
\end{aligned}$$

$(-1$

GIVEN $f\in\mathbb{A}$;
FIND, in case of existence, a $g\in\mathbb{A}$ such that

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

s $\dots,p_e)[x]$

$\dots,p_e)[x][s_1]$

$$\sigma(s_3) = s_3+f_3 \quad f_3\in\mathbb{K}(k)(p_1,\dots,p_e)[x][s_1][s_2]$$

$$\vdots$$

such that $\mathrm{const}_\sigma\mathbb{A} = \{c\in\mathbb{A}\,|\,\sigma(c)=c\}=\mathbb{K}$.

Telescoping in the given difference ring

FIND a closed form for

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

A $R\Pi\Sigma^*$-ring for the summand $\boxed{\mathrm{const}_\sigma \mathbb{A} = \mathbb{Q}}$

Consider a ring

$$\mathbb{A} := \mathbb{Q}(k)[h]$$

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

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

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

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

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

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

Degree bound: COMPUTE $b \geq 0$:

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

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

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

Degree bound: COMPUTE $b \geq 0$: $\boxed{b = 2}$

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

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

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

Degree bound: COMPUTE $b \geq 0$: $\boxed{b = 2}$

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

Polynomial Solution: FIND

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

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

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

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

$$\begin{aligned}&\big[\sigma(g_2\,h^2 + g_1 h + g_0)\big]\\ &\qquad\qquad -\big[g_2\,h^2 + g_1 h + g_0\big] = h\end{aligned}$$

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

$$\begin{aligned}&\Big[\sigma(g_2\, h^2) + \sigma(g_1 h + g_0)\Big]\\ &\qquad\qquad -\Big[g_2\, h^2 + g_1 h + g_0\Big] = h\end{aligned}$$

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

$$\big[\sigma(g_2)\,\sigma(h^2) + \sigma(g_1 h + g_0)\big] \\ -\big[g_2\, h^2 + g_1 h + g_0\big] = h$$

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

$$\begin{aligned}\big[\sigma(g_2)\,\sigma(h)^2 + \sigma(g_1 h + g_0)\big]&\\ -\big[g_2\, h^2 + g_1 h + g_0\big] &= h\end{aligned}$$

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

$$\begin{aligned}\Big[\sigma(g_2)\big(h+\tfrac{1}{k+1}\big)^2 + \sigma(g_1 h + g_0)\Big]&\\ -\Big[g_2\, h^2 + g_1 h + g_0\Big] &= h\end{aligned}$$

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

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coeff. comp. $\boxed{}$

$$\boxed{\sigma(g_2) - g_2 = 0}$$

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

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

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$$\boxed{\sigma(g_2)-g_2=0}$$

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

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

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coeff. comp.

$$\boxed{\sigma(g_2)-g_2=0}$$

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

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

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

coeff. comp.

$$\boxed{\sigma(g_2) - g_2 = 0}$$

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

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

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

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

coeff. comp.

$$\boxed{\sigma(g_2) - g_2 = 0}$$

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

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

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

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

coeff. comp. $\boxed{}$

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

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

coeff. comp.

$$\boxed{\sigma(g_1) - g_1 = 1 - c\,\frac{2}{k+1}}$$

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

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

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$$\boxed{\sigma(g_1) - g_1 = 1 - c\,\tfrac{2}{k+1}}$$

$c = 0$, $\begin{array}{l} g_1 = k + d \\ d \in \mathbb{Q} \end{array}$

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

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

coeff. comp.

$$\boxed{\sigma(g_2) - g_2 = 0}$$

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

coeff. comp.

$$\boxed{\sigma(g_1) - g_1 = 1 - c\,\tfrac{2}{k+1}}$$

$c = 0,$ $\quad g_1 = k + d$, $d \in \mathbb{Q}$

$$\boxed{\sigma(g_0) - g_0 = -1 - d\frac{1}{k+1}}$$

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

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

coeff. comp.

g=hk-k

$$\boxed{\sigma(g_2) - g_2 = 0}$$

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

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

coeff. comp.

$$\boxed{\sigma(g_1) - g_1 = 1 - c\,\tfrac{2}{k+1}}$$

$c = 0$, $\begin{array}{l} g_1 = k + d \\ d \in \mathbb{Q} \end{array}$

$$\begin{array}{l} g_0 = -k \\ d = 0 \end{array} \quad \leftarrow \quad \boxed{\sigma(g_0) - g_0 = -1 - d\frac{1}{k+1}}$$

Telescoping in the given difference ring

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

$$\boxed{\sigma(g) - g = h.}$$

We compute

$$g = (h-1)k \in \mathbb{A}.$$

This gives

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

with

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

Hence,

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

Toolbox 1: Improved indefinite summation – symbolic simplification

For algorithmic details see:

- CS. Symbolic summation with single-nested sum extensions. In J. Gutierrez, editor, *Proc. ISSAC'04*, pages 282–289. ACM Press, 2004.
- CS. Product representations in $\Pi\Sigma$-fields. *Ann. Comb.*, 9(1):75–99, 2005.
- CS. Simplifying Sums in $\Pi\Sigma$-Extensions. *J. Algebra Appl.*, 6(3):415–441, 2007.
- CS. A refined difference field theory for symbolic summation. *J. Symbolic Comput.*, 43(9):611–644, 2008. [arXiv:0808.2543v1].
- S.A. Abramov, M. Petkovšek. Polynomial ring automorphisms, rational (w, σ)-canonical forms, and the assignment problem. *J. Symbolic Comput.*, 45(6): 684–708, 2010.
- CS, A Symbolic Summation Approach to Find Optimal Nested Sum Representations. In: A. Carey, D. Ellwood, S. Paycha, S. Rosenberg (eds.) Motives, Quantum Field Theory, and Pseudodifferential Operators, Clay Mathematics Proceedings, vol. 12, pp. 285–308. Amer. Math. Soc (2010). ArXiv:0808.2543
- CS, Parameterized Telescoping Proves Algebraic Independence of Sums. Ann. Comb. **14**(4), 533–552 (2010). [arXiv:0808.2596]
- CS. Structural Theorems for Symbolic Summation. *Appl. Algebra Engrg. Comm. Comput.*, 21(1):1–32, 2010.
- CS. Fast Algorithms for Refined Parameterized Telescoping in Difference Fields. To appear in *Computer Algebra and Polynomials*, Lecture Notes in Computer Science (LNCS), Springer, 2014. arXiv:1307.7887 [cs.SC].

For special cases see:

- S.A. Abramov. On the summation of rational functions. Zh. vychisl. mat. Fiz., 11: 1071-1074, 1971.
- P. Paule. Greatest factorial factorization and symbolic summation, J. Symbolic Comput., 20(3): 235-268, 1995.

The basic difference ring approach

GIVEN a $R\Pi\Sigma^*$-ring/$\Pi\Sigma^*$-field $(\mathbb{A},\sigma)$ with $f\in\mathbb{A}$.

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

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

A symbolic summation approach

1. FIND an appropriate $R\Pi\Sigma^*$-ring/$\Pi\Sigma^*$-field $(\mathbb{A}, \sigma)$ with $f \in \mathbb{A}$.

2. FIND $g \in \mathbb{A}$:

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

A symbolic summation approach

1. FIND an appropriate $R\Pi\Sigma^*$-ring/$\Pi\Sigma^*$-field $(\mathbb{A}, \sigma)$ with $f \in \mathbb{A}$.

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appropriate = degrees in denominators minimal

Example:

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

$$=?$$

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

A symbolic summation approach

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

appropriate = sum representations with optimal nesting depth

Example:

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

A symbolic summation approach

1. FIND an appropriate $R\Pi\Sigma^*$-ring/$\Pi\Sigma^*$-field $(\mathbb{A},\sigma)$ with $f\in\mathbb{A}$.

2. FIND an appropriate extension $\mathbb{E}>\mathbb{A}$ with $g\in\mathbb{E}$:
$$\sigma(g)-g=f.$$

appropriate = sum representations with optimal nesting depth

Example:

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

depth 3 depth 1

Simplification of nested product-sum expressions

$\boxed{A(k)\text{: nested product-sum expression (sums/products not in the denominator)}}$

$$\downarrow \quad \texttt{SigmaReduce[A,k]}$$

$\boxed{B(k)\text{: nested product-sum expression (sums/products not in the denominator)}}$

- such that

$$A(\lambda) = B(\lambda) \qquad\qquad \text{for almost all } \lambda \in \mathbb{N}$$

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- such that

$$A(\lambda) = B(\lambda) \qquad\qquad \text{for almost all } \lambda \in \mathbb{N}$$

- such that all the sums in $B(k)$ are **simplified** as above
- and such that the arising sums in $B(k)$ are **algebraically independent** (i.e., they do not satisfy any polynomial relation)

Toolbox 2: Definite summation

$$(n+2)\mathbf{A}(n+1) - n\mathbf{A}(n) = \frac{(n+1)S_1(n)+1}{(n+1)^3}$$

Summation package Sigma

(based on difference field/ring algorithms/theory
see, e.g., Karr 1981, Bronstein 2000, Schneider 2001/2004/2005a–c/2007/2008/2010a–c)

$$\boxed{A(n) = \sum_{k=1}^{\infty} \frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)}} = \boxed{{\color{blue}0} \times \frac{1}{n(n+1)} + \frac{S_1(n)^2+S_2(n)}{2n(n+1)}}$$

where

$$S_1(n) = \sum_{i=1}^{n} \frac{1}{i} \qquad S_2(n) = \sum_{i=1}^{n} \frac{1}{i^2}$$

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 $A(n)$

Zeilberger's creative telescoping paradigm

GIVEN
$$\mathsf{A}(n) := \sum_{k=1}^{a} \underbrace{\frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)}}_{=:\, f(n,k)}.$$

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

Sigma *computes*: $c_0(n) = -n$, $c_1(n) = (n+2)$ and

$$g(n,k) = \frac{kS_1(k)+(-n-1)S_1(n)-kS_1(k+n)-2}{(k+n+1)(n+1)^2}$$

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for all $0 \le k \le n$ and all $n \ge 0$.

Summing this equation over k from 1 to a gives:

$$\boxed{g(n,a+1)-g(n,1)} = \boxed{c_0(n)\,\mathsf{A}(n)+c_1(n)\,\mathsf{A}(n+1)}$$

$$\begin{array}{ccc} || & & || \\ \frac{(a+1)(S_1(a)+S_1(n)-S_1(a+n))}{(n+1)^2(a+n+2)} + \frac{a(a+1)}{(n+1)^3(a+n+1)(a+n+2)} & & -n\mathsf{A}(n)+(2+n)\mathsf{A}(n+1) \end{array}$$

Zeilberger's creative telescoping paradigm

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

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

Summing this equation over k from 1 to a gives:

$$\begin{array}{ccc} \boxed{g(n,a+1)-g(n,1)} & = & \boxed{c_0(n)\,\mathsf{A}(n) + c_1(n)\,\mathsf{A}(n+1)} \\ \lim_{a\to\infty} \| & & \| \\ \dfrac{(n+1)S_1(n)+1}{(n+1)^3} & & -n\mathsf{A}(n) + (2+n)\mathsf{A}(n+1) \end{array}$$

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

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2. Recurrence solving

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

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

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

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(d'Alembertian solutions)
(Abramov/Bronstein/Petkovšek/CS, in preparation)

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

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FIND all solutions expressible by indefinite nested products/sums in n.
(d'Alembertian solutions)
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4. Find a "closed form"

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

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

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

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

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Compute a recurrence

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

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

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

Out[4]= $$-\mathtt{n}\mathsf{SUM}[\mathtt{n}] + (1+\mathtt{n})(2+\mathtt{n})\mathsf{SUM}[\mathtt{n}+1] == \frac{(\mathtt{n}+1)\mathtt{S}_1(\mathtt{n})+1}{(\mathtt{n}+1)^3}$$

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Solve a recurrence

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

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

Out[4]= $$-n\mathsf{SUM}[n] + (1+n)(2+n)\mathsf{SUM}[n+1] == \frac{(n+1)S_1(n)+1}{(n+1)^3}$$

Solve a recurrence

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

Out[5]= $$\{\{0, \frac{1}{n(n+1)}\}, \{1, \frac{\sum_{i=1}^{n} \frac{S_1(i)}{i}}{n(n+1)}\}\}$$

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

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

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Compute a recurrence

In[3]:= **rec = GenerateRecurrence[mySum, n][[1]]**

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

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

Out[4]= $$-\mathtt{n}\mathsf{SUM}[\mathtt{n}] + (1+\mathtt{n})(2+\mathtt{n})\mathsf{SUM}[\mathtt{n}+1] == \frac{(\mathtt{n}+1)\mathtt{S}_1(\mathtt{n})+1}{(\mathtt{n}+1)^3}$$

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Solve a recurrence

In[5]:= **recSol = SolveRecurrence[rec, SUM[n], IndefiniteSummation → True]**

Out[5]= $$\{\{0, \frac{1}{n(n+1)}\}, \{1, \frac{S_1(n)^2 + \sum_{i=1}^{n} \frac{1}{i^2}}{2n(n+1)}\}\}$$

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

Out[4]= $-n\mathsf{SUM}[n]+(1+n)(2+n)\mathsf{SUM}[n+1] == \frac{(n+1)S_1(n)+1}{(n+1)^3}$

Solve a recurrence

In[5]:= **recSol = SolveRecurrence[rec, SUM[n], IndefiniteSummation → True]**

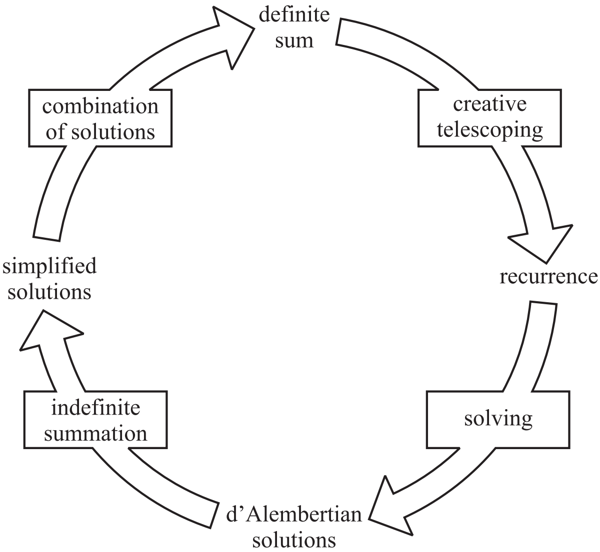
Out[5]= $\{\{0, \frac{1}{n(n+1)}\}, \{1, \frac{S_1(n)^2+\sum_{i=1}^{n}\frac{1}{i^2}}{2n(n+1)}\}\}$

Combine the solutions

In[6]:= **FindLinearCombination[recSol, {1, {1/2}, n, 2]**

Out[6]= $\frac{S_1(n)^2+\sum_{i=1}^{n}\frac{1}{i^2}}{2n(n+1)}$

Sigma's summation spiral



Toolbox 3: Special function algorithms

Computer algebra and special functions:

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

$$\boxed{\sum_{i=1}^{n} \frac{1}{i^2} \sum_{j=1}^{i} \frac{1}{j}}$$

Computer algebra and special functions:

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

$$\boxed{\sum_{i=1}^{n}\frac{1}{i^2}\sum_{j=1}^{i}\frac{1}{j}}$$

Integral representation:

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

Computer algebra and special functions:

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

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Integral representation:

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

Asymptotic expansion:

$$=\left(\frac{1}{30n^5}-\frac{1}{6n^3}+\frac{1}{2n^2}-\frac{1}{n}\right)\ln(n)$$

$$-\tfrac{1}{100n^5}-\tfrac{1}{6n^4}+\tfrac{13}{36n^3}-\tfrac{1}{4n^2}-\tfrac{1}{n}+2\zeta_3+O(\tfrac{\ln(n)}{n^6}).$$

limit computations **numerical evaluation**

- Generalized algorithms for generalized harmonic sums

$$\sum_{k=1}^{N}\frac{2^k\sum_{i=1}^{k}\frac{2^{-i}\sum_{j=1}^{i}\frac{S_1(j)}{j}}{i}}{k} = -\frac{21\zeta_2^2}{20}\frac{1}{N}+\frac{1}{8N^2}+\frac{295}{216N^3}-\frac{1115}{96N^4}+O(N^{-5}$$

$$+\Big(\frac{1}{2N}-\frac{3}{4N^2}+\frac{19}{12N^3}-\frac{5}{N^4}+O(N^{-5})\Big)\zeta_2$$

$$+2^N\Big(\frac{3}{2N}+\frac{3}{2N^2}+\frac{9}{2N^3}+\frac{39}{2N^4}+O(N^{-5})\Big)\zeta_3$$

$$+\Big(\frac{1}{N}+\frac{3}{4N^2}-\frac{157}{36N^3}+\frac{19}{N^4}+O(N^{-5})\Big)(\log(N)+\gamma)$$

$$+\Big(\frac{1}{2N}-\frac{3}{4N^2}+\frac{19}{12N^3}-\frac{5}{N^4}+O(N^{-5})\Big)(\log(N)+\gamma)^2)$$

[Ablinger, Blümlein, CS, J. Math. Phys. 54, 2013, arXiv:1302.0378 [math-ph]]

- Generalized algorithms for cyclotomic harmonic sums

$$
\begin{aligned}
\sum_{k=1}^{N} \frac{\displaystyle\sum_{j=1}^{k} \frac{\displaystyle\sum_{i=1}^{j} \frac{1}{1+2i}}{j^2}}{(1+2k)^2} =& \Big(-3+\frac{35\zeta_3}{16}\Big)\zeta_2 - \frac{31\zeta_5}{8} \\
&+ \frac{1}{N} - \frac{33}{32N^2} + \frac{17}{16N^3} - \frac{4795}{4608N^4} + O(N^{-5}) \\
&+ \log(2)\Big(6\zeta_2 - \frac{1}{N} + \frac{9}{8N^2} - \frac{7}{6N^3} + \frac{209}{192N^4} + O(N^{-5})\Big) \\
&+ \Big(-\frac{7}{4} - \frac{7}{16N} + \frac{7}{16N^2} - \frac{77}{192N^3} + \frac{21}{64N^4} + O(N^{-5})\Big)\zeta_3 \\
&+ \Big(\frac{1}{16N^2} - \frac{1}{8N^3} + \frac{65}{384N^4} + O(N^{-5})\Big)(\log(N)+\gamma)
\end{aligned}
$$

[Ablinger, Blümlein, CS, J. Math. Phys. 52, 2011, arXiv:1302.0378 [math-ph]]

- Generalized algorithms for nested binomial sums

$$
\begin{aligned}
\sum_{j=1}^{N} \frac{4^j S_1(j-1)}{\binom{2j}{j} j^2} = 7\zeta_3 + \sqrt{\pi}\sqrt{N}\Bigg\{ \Bigg[& -\frac{2}{N} + \frac{5}{12N^2} - \frac{21}{320N^3} - \frac{223}{10752N^4} + \frac{671}{49152N^5} \\
& + \frac{11635}{1441792N^6} - \frac{1196757}{136314880N^7} - \frac{376193}{50331648N^8} + \frac{201980317}{18253611008N^9} \\
& + O(N^{-10}) \Bigg] \ln(\bar{N}) - \frac{4}{N} + \frac{5}{18N^2} - \frac{263}{2400N^3} + \frac{579}{12544N^4} + \frac{10123}{1105920N^5} \\
& - \frac{1705445}{71368704N^6} - \frac{27135463}{11164188672N^7} + \frac{197432563}{7927234560N^8} + \frac{405757489}{775778467840N^9} \\
& + O(N^{-10}) \Bigg\}
\end{aligned}
$$

Ablinger, Blümlein, CS, ACAT 2013, arXiv:1310.5645 [math-ph]

Ablinger, Blümlein, Raab, CS, J. Math. Phys. 55, 2014. arXiv:1407.1822 [hep-th]

The full machinery:

Toolbox 1 + Toolbox 2 + Toolbox 3

The full machinery:

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

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

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

HarmonicSums by Jakob Ablinger © RISC-Linz

In[3]:= $<<$ **EvaluateMultiSums.m**

EvaluateMultiSums by Carsten Schneider © RISC-Linz

In[4]:= **EvaluateMultiSum**[

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Big(\frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!}\Big), \{n\}, \{1\}]$$

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$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Big(\frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!}\Big), \{n\}, \{1\}]$$

Out[4]= $\dfrac{S_1(n)^2+3S_2(n)}{2n(n+1)!}$

Can we trust these calculations?

Can we trust these calculations?

- Steps can be verified by proof certificates:
  - telescoping

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\underbrace{\Big(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}\Big)}_{f(j)}$$

FIND $g(j)$:

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

$\uparrow$ summation package Sigma

$$g(j) = \frac{(j+k+1)(j+n+1)j!k!(j+k+n)!\Big(S_1(j)-S_1(j+k)-S_1(j+n)+S_1(j+k+n)\Big)}{kn(j+k+1)!(j+n+1)!(k+n+1)!}$$

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FIND $g(j)$:

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

Summing the telescoping equation over j from 0 to a gives

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

$$=\frac{(a+1)!(k-1)!(a+k+n+1)!(S_1(a)-S_1(a+k)-S_1(a+n)+S_1(a+k+n))}{n(a+k+1)!(a+n+1)!(k+n+1)!}$$

$$\underbrace{+\frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)n!}+\frac{(2a+k+n+2)a!k!(a+k+n)!}{(a+k+1)(a+n+1)(a+k+1)!(a+n+1)!(k+n+1)!}}$$

$a \to \infty$

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Big(\underbrace{\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}}_{f(j)}\Big)$$

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

$$\overset{a\to\infty}{=} \frac{1}{n!}\,\frac{S_1(k)+S_1(n)-S_1(k+n)}{kn(k+n+1)}$$

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  - creative telescoping

Zeilberger's creative telescoping paradigm

GIVEN

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

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

Sigma *computes*: $c_0(n) = -n$, $c_1(n) = (n+2)$ and

$$g(n,k) = \frac{kS_1(k) + (-n-1)S_1(n) - kS_1(k+n) - 2}{(k+n+1)(n+1)^2}$$

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for all $0 \le k \le n$ and all $n \ge 0$.

Summing this equation over k from 1 to a gives:

$$\boxed{g(n,a+1) - g(n,1)} = \boxed{c_0(n)\,\mathsf{A}(n) + c_1(n)\,\mathsf{A}(n+1)}$$

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

$$\frac{(a+1)(S_1(a)+S_1(n)-S_1(a+n))}{(n+1)^2(a+n+2)} + \frac{a(a+1)}{(n+1)^3(a+n+1)(a+n+2)} \qquad -n\mathsf{A}(n) + (2+n)\mathsf{A}(n+1)$$

Zeilberger's creative telescoping paradigm

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$$\begin{array}{ccc} \boxed{g(n,a+1)-g(n,1)} & = & \boxed{c_0(n)\,\mathsf{A}(n) + c_1(n)\,\mathsf{A}(n+1)} \\ \lim\limits_{a\to\infty} \| & & \| \\ \dfrac{(n+1)S_1(n)+1}{(n+1)^3} & & -\,n\mathsf{A}(n) + (2+n)\mathsf{A}(n+1) \end{array}$$

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Summation controlled by proof certificates

$$\sum_{k=a}^{b} f(n,k)$$

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closed form for
missing summation points

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$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\underbrace{\Big(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}\Big)}_{f(j)}$$

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- Steps are based on limit calculations...
  - ... on symbolic methods verified by analysis

Computer algebra and special functions:

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

$$\boxed{\sum_{i=1}^{n}\frac{1}{i^2}\sum_{j=1}^{i}\frac{1}{j}}$$

Integral representation:

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

Asymptotic expansion:

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

limit computations **numerical evaluation**

Can we trust these calculations?

- Steps can be verified by proof certificates:
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- Steps are controlled by proof certificates
- Steps are based on limit calculations...
  - ... on symbolic methods verified by analysis
  - ... on table look-ups (for speed-ups)

    $\rightarrow$ entries can be verified independently

Can we trust these calculations? YES

- Steps can be verified by proof certificates:
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Example 1: A bet on my cost

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:
```

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

[Arose in the analysis of the simplex algorithm on the Klee-Minty cube (J. Balogh, R. Pemantle)]

In[5]:= $\mathbf{EvaluateMultiSum}[\sum_{n=1}^{\infty}\sum_{k=1}^{\infty}\frac{S_1(k)(S_1(n+1)-1)}{kn(n+1)(k+n)}]$

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Out[5]= $-4\zeta_2 - 2\zeta_3 + 4\zeta_2\zeta_3 + 2\zeta_5$

$60s <$ in a jiffy

In[5]:= $\mathbf{EvaluateMultiSum}[\sum_{n=1}^{\infty}\sum_{k=1}^{\infty}\frac{S_1(k)(S_1(n+1)-1)}{kn(n+1)(k+n)}]$

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$60s <$ in a jiffy

$=0.999222...$

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Produce variations:

In[6]:= $\mathbf{EvaluateMultiSum}[\sum_{n=1}^{\infty}\sum_{k=1}^{\infty}\frac{S_1(k)^2(S_1(n+1)-1)^2}{k\,(k+n)\,n}]$

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Out[6]= $-10\zeta_3 + \zeta_2^2\left(\frac{58\zeta_3}{5} - \frac{29}{5}\right) - 10\zeta_5 + \zeta_2(-\zeta_3 + 13\zeta_5 - 4) + \frac{457\zeta_7}{8}$

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In[7]:= $\mathbf{EvaluateMultiSum}[\sum_{n=1}^{\infty}\sum_{k=1}^{\infty}\frac{S_1(k)(S_1(n+1)-1)}{k\,(k+n)^2n^2}]$

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Out[7]= $2\zeta_3+\zeta_2^2\left(\frac{17\zeta_3}{10}+\frac{17}{10}\right)+\zeta_2(2\zeta_3-3\zeta_5-4)-\frac{9\zeta_5}{2}+\frac{3\zeta_7}{16}$

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Out[5]= $-4\zeta_2 - 2\zeta_3 + 4\zeta_2\zeta_3 + 2\zeta_5$

Produce variations:

In[6]:= $\mathbf{EvaluateMultiSum}[\sum_{n=1}^{\infty}\sum_{k=1}^{\infty}\frac{S_1(k)^2(S_1(n+1)-1)^2}{k\,(k+n)\,n}]$

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In[8]:= $\mathbf{EvaluateMultiSum}[\sum_{n=1}^{\infty}\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{S_1(k)S_1(n)S_1(n+l+k)}{k\,(k+n)\,(k+n+l+1)^2}]$

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Out[6]= $-10\zeta_3+\zeta_2^2\left(\frac{58\zeta_3}{5}-\frac{29}{5}\right)-10\zeta_5+\zeta_2(-\zeta_3+13\zeta_5-4)+\frac{457\zeta_7}{8}$

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Out[8]= $3\zeta_3^2-\frac{15\zeta_5}{2}+\zeta_2(9\zeta_5-6\zeta_3)+\frac{149\zeta_7}{16}+\frac{114}{35}\zeta_2^3$

Example 2: The Stam project

(joint with B. Buchberger, P. Paule, C. Koutschan, W. Windsteiger,. . .)

$\rightarrow$ Bruno Buchberger's talk on Monday

Binomial identities with old-fashioned proofs by A.J. Stam; page 1055:

$$(6.8) \qquad \sum_{k=0}^{2n} (-1)^k \binom{2n}{k}^3 = \frac{(-1)^n (3n)!}{(n!)^3} \qquad \text{(Dixon's identity)}$$

Binomial identities with old-fashioned proofs by A.J. Stam; page 1055:

$$\sum_{k=0}^{2n}(-1)^k\binom{2n}{k}^3=\frac{(-1)^n(3n)!}{(n!)^3} \tag{6.8}$$

(Dixon's identity)

Find Dixon's identity:

In[9]:= $\mathbf{EvaluateMultiSum}[\sum_{k=0}^{2n}(-1)^k\binom{2n}{k}^3,\{n\},\{1\}]$

Out[9]= $\frac{(-1)^n(3n)!}{(n!)^3}$

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$$(6.8) \qquad \sum_{k=0}^{2n}(-1)^k\binom{2n}{k}^3 = \frac{(-1)^n(3n)!}{(n!)^3} \qquad \text{(Dixon's identity)}$$

Find new identities:

In[9]:= $\mathbf{EvaluateMultiSum}[\sum_{\mathbf{k=0}}^{\mathbf{2n}}(\mathbf{-1})^{\mathbf{k}}\binom{\mathbf{2n}}{\mathbf{k}}^{\mathbf{3}}\mathbf{S_1(k), \{n\}, \{1\}}]$

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Find new identities:

In[9]:= $\mathbf{EvaluateMultiSum}[\sum_{k=0}^{2n}(-1)^k\binom{2n}{k}^3 S_1(k), \{n\}, \{1\}]$

Out[9]= $\frac{(-1)^n(3n)!}{(n!)^3}\left(\frac{1}{2}S_1(n)+S_1(2n)-\frac{1}{2}S_1(3n)\right)$

Binomial identities with old-fashioned proofs by A.J. Stam; page 1055:

$$(6.8) \qquad \sum_{k=0}^{2n}(-1)^k\binom{2n}{k}^3=\frac{(-1)^n(3n)!}{(n!)^3} \qquad \text{(Dixon's identity)}$$

Find new identities:

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Find new identities:

In[9]:= $\mathbf{EvaluateMultiSum}[\sum_{k=0}^{2n}(-1)^k\binom{2n}{k}^3 S_1(k)^2, \{n\}, \{1\}]$

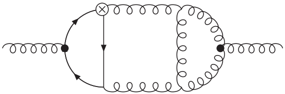
Out[9]= $\frac{(-1)^n(3n)!}{(n!)^3}\frac{1}{12}\left(3\left(S_1(n)+2S_1(2n)-S_1(3n)\right)^2-S_2(n)+2S_2(2n)-3S_2(3n)\right)$

Example 3: Feynman integrals

joint work with J. Ablinger, A. Behring, J. Blümlein, A. Hasselhuhn, A. de Freitas, C. Raab, M. Round, F. Wissbrock (RISC–DESY)

Evaluation of Feynman diagrams

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



Behavior of particles

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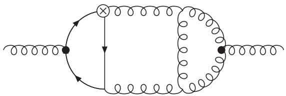


Behavior of particles

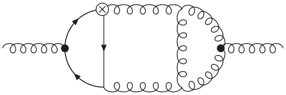
$$\longrightarrow$$

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

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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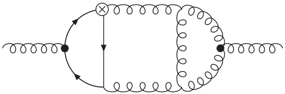

Behavior of particles

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

Feynman integrals

$\downarrow$ **DESY**

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

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simple sum expressions $\xleftarrow{\textbf{symbolic summation}}$ multi sums

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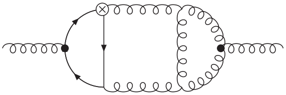


Behavior of particles

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

Feynman integrals

DESY

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

multi sums

symbolic summation

simple sum expressions

processable by physicists

Evaluations required for the
LHC experiment at CERN

A warm-up example: simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Big(\underbrace{\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} + \frac{j!k!(j+k+n)!\,(-S_1(j)+S_1(j+k)+S_1(j+n)-S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!}}\Big)$$

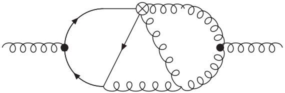
$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f(n,k,j) = \frac{S_1(n)^2+3S_2(n)}{2n(n+1)!}$$

where

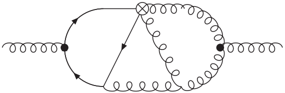
$$S_1(n)=\sum_{i=1}^{n}\frac{1}{i} \qquad S_2(n)=\sum_{i=1}^{n}\frac{1}{i^2}$$

Arose in the context of

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



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



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

Simplify

$$\|$$

$$\boxed{\begin{aligned}&\sum_{j=0}^{n-3}\sum_{k=0}^{j}\sum_{l=0}^{k}\sum_{q=0}^{-j+n-3}\sum_{s=1}^{-l+n-q-3}\sum_{r=0}^{-l+n-q-s-3}(-1)^{-j+k-l+n-q-3}\times\\ &\times\frac{\binom{j+1}{k+1}\binom{k}{l}\binom{n-1}{j+2}\binom{-j+n-3}{q}\binom{-l+n-q-3}{s}\binom{-l+n-q-s-3}{r}r!(-l+n-q-r-s-3)!(s-1)!}{(-l+n-q-2)!(-j+n-1)(n-q-r-s-2)(q+s+1)}\\ &\Big[4S_1(-j+n-1)-4S_1(-j+n-2)-2S_1(k)\\ &-(S_1(-l+n-q-2)+S_1(-l+n-q-r-s-3)-2S_1(r+s))\\ &+2S_1(s-1)-2S_1(r+s)\Big] + \textbf{3 further 6–fold sums}\end{aligned}}$$

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

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

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

$$+\Big(- \ldots 1)^N(2N+1) \ldots N(N+1) - \frac{13}{N}\Big)S_2(N) + \Big(\frac{29}{3} - (-1)^N\Big)S_3(N)$$

$$+\big(2 + \ldots 28S_{-2,1}(N) + \frac{20(-1)^N}{N^2(N+1)}\big)S_1(N) + \Big(\frac{3}{4} + (-1)^N\Big)S_2(N)^2$$

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$$+\Big(\frac{(-1)^N(5-3N)}{2N^2(N+1)} - \frac{5}{2N^2}\Big)S_2(N) + S_{-2}(N)\Big(10S_1(N)^2 + \Big(\frac{8(-1)^N(2N+1)}{N(N+1)}$$

$$+\frac{4(3N-1)}{N(N+1)}\Big)S_1(N) + \frac{8(-1)^N(3N+1)}{N(N+1)^2} + \big(-22 + 6(-1)^N\big)S_2(N) - \frac{16}{N(N+1)}\Big)$$

$$+\Big(\frac{(-1)^N(9N+5)}{N(N+1)} - \frac{29}{3N}\Big)S_3(N) + \Big(\frac{19}{2} - 2(-1)^N\Big)S_4(N) + \big(-6 + 5(-1)^N\big)S_{-4}(N)$$

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$$+ \Big(\frac{(-1)^N(5-3N)}{2N^2 \cdots} - \frac{5}{\cdots}\Big)S_2(N) + S_{-2}(N)\Big(10S_1(N)^2 + \Big(\frac{\cdots(2N+1)}{N(N+1)}$$

$$+ \frac{4(3N - \cdots}{N(N + \cdots} \cdots -1)^N\big)S_2(N) - \frac{16}{N(N+1)}\Big)$$

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So far derived results (see Nucl. Phys. B and Phys. Review D)

1. I. Bierenbaum, J. Blümlein, S. Klein, and C. Schneider. Two–Loop Massive Operator Matrix Elements for Unpolarized Heavy Flavor Production to $O(\epsilon)$. *Nucl.Phys. B* 803(1-2):1–41, 2008.
2. J. Ablinger, J. Blümlein, S. Klein, C. Schneider, F. Wissbrock. The $O(\alpha_s^3)$ Massive Operator Matrix Elements of $O(n_f)$ for the Structure Function $F_2(x, Q^2)$ and Transversity. Nucl. Phys. B, 844: 26-54, 2011.
3. J. Ablinger, J. Blümlein, A. Hasselhuhn, S. Klein, C. Schneider, F. Wissbrock Massive 3-loop Ladder Diagrams for Quarkonic Local Operator Matrix Elements. Nuclear Physics B. 864: 52-84, 2012.
4. J. Blümlein, A. Hasselhuhn, S. Klein, C. Schneider. The $O(\alpha_s^3 n_f T_F^2 C_{A,F})$ Contributions to the Gluonic Massive Operator Matrix Elements. Nuclear Physics B: 866: 196-211, 2013.
5. J. Ablinger, J. Blümlein, A. De Freitas A. Hasselhuhn, A. von Manteuffel, M. Round, C. Schneider, F. Wissbrock. The Transition Matrix Element $A_{gq}(N)$ of the Variable Flavor Number Scheme at $O(\alpha_s^3)$. Nuclear Physics B 882, pp. 263-288. 2014.
6. J. Ablinger, J. Blümlein, C. Raab, C. Schneider, F. Wissbrock. Calculating Massive 3-loop Graphs for Operator Matrix Elements by the Method of Hyperlogarithms. Nuclear Physics B 885, pp. 409-447. 2014.
7. J. Ablinger, J. Blümlein, A. De Freitas, A. Hasselhuhn, A. von Manteuffel, M. Round, C. Schneider. The $O(\alpha_s^3 T_F^2)$ Contributions to the Gluonic Operator Matrix Element. Nuclear Physics B 885, pp. 280-317. 2014.
8. J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. Hasselhuhn, A. von Manteuffel, M. Round, C. Schneider, F. Wissbrock. The 3-Loop Non-Singlet Heavy Flavor Contributions and Anomalous Dimensions for the Structure Function $F_2(x, Q^2)$ and Transversity. Nuclear Physics B 886, pp. 733-823. 2014.
9. J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel, C. Schneider The 3-Loop Pure Singlet Heavy Flavor Contributions to the Structure Function $F_2(x, Q^2)$ and the Anomalous Dimension. Nuclear Physics B 890, pp. 48-151. 2015. arXiv:1409.1135 [hep-ph].
10. A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel, C. Schneider. The 3-Loop Non-Singlet Heavy Flavor Contributions to the Structure Function $g_1(x, Q^2)$ at Large Momentum Transfer. Nucl. Phys. B 897, pp. 612-644. 2015. arXiv:1504.08217 [hep-ph].
11. A. Behring, J. Blümlein, A. De Freitas, A. Hasselhuhn, A. von Manteuffel, C. Schneider. The $O(\alpha_s^3)$ Heavy Flavor Contributions to the Charged Current Structure Function $xF_3(x, Q^2)$ at Large Momentum Transfer. Physical Review D 92(114005), pp. 1-19. 2015. arXiv:1508.01449 [hep-ph].

So far derived results (see Nucl. Phys. B and Phys. Review D)

Determine the coupling constant of the strong force
(5 % error → 1% error)

One (of many) motivations:
the central value hints if and how the
fundamental forces unite to one elementary force

1. I. Bierenbaum, J. Blümlein, S. Klein, and C. Schneider. Two–Loop Massive Operator Matrix Elements for Unpolarized Heavy Flavor Production to $O(\epsilon)$. *Nucl.Phys. B* 80[illegible](1-2):1–41, 2008.
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- reliable software based on proof certificates