Waterloo, Canada, July 22, 2016

ISSAC 2016

Symbolic summation in difference rings and applications

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FWF Der Wissenschaftsfonds

Some of the available summation tools:

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- M. Kauers and P. Paule. *The concrete tetrahedron*. Texts and Monographs in Symbolic Computation. SpringerWienNewYork, Vienna, 2011. Symbolic sums, recurrence equations, generating functions, asymptotic estimates.

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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)
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- 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)
- Pirastu, R., Strehl, V.: Rational summation and Gosper-Petkovšek representation. J. Symbolic Comput. **20**(5-6), 617–635 (1995)
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Here I will restrict to the setting of difference rings/fields.

A warm-up example: simplify

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

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

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

FIND $g(j)$:

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

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 $g(j)$:

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

↑ 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

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

FIND $g(j)$:

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Summing the telescoping equation over j from 0 to a gives

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

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

A warm-up example: simplify

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

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

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

no solution ☹

Zeilberger's creative telescoping paradigm

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

FIND $g(n,k)$

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

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

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

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

Summing this equation over k from 1 to a gives:

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

Zeilberger's creative telescoping paradigm

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Summing this equation over k from 1 to a gives:

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

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

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

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

recurrence finder

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

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

recurrence solver

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

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–)

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

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

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

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

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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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 $(\mathbb{A}, \sigma)$ for $f(k)$:

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

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

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

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

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$$\boxed{\mathbb{A} := \mathbb{K}(k)[p_1, p_1^{-1}]}$$

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

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hypergeometric	$\leftrightarrow$	$\sigma(p_1) = a_1\, p_1$	$a_1 \in \mathbb{K}(k)^*$
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$$\boxed{\mathbb{A} := \mathbb{K}(k)[p_1, p_1^{-1}][p_2, p_2^{-1}] \dots [p_e, p_e^{-1}]}$$

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

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

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$$\boxed{\mathbb{A} := \mathbb{K}(k)[p_1,p_1^{-1}][p_2,p_2^{-1}]\dots[p_e,p_e^{-1}][x]}$$

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

$$\mathbf{(-1)^k} \quad \leftrightarrow \quad \sigma(\mathbf{x}) = -\mathbf{x} \qquad \mathbf{x^2=1}$$

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α is a primitive λth root of unity $\quad \alpha^{\mathbf{k}} \quad \leftrightarrow \quad \sigma(\mathbf{x}) = \alpha\, \mathbf{x} \qquad \mathbf{x}^{\lambda} = \mathbf{1}$

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$$\mathbb{A} := \mathbb{K}(k)[p_1, p_1^{-1}][p_2, p_2^{-1}] \dots [p_e, p_e^{-1}][x][s_1]$$

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α is a primitive λth root of unity $\alpha^{\mathbf{k}}$	$\leftrightarrow$	$\sigma(\mathbf{x}) = \alpha\, \mathbf{x}$	$\mathbf{x}^{\lambda} = \mathbf{1}$
$\mathcal{S} S_1(k) = S_1(k) + \frac{1}{k+1}$	$\leftrightarrow$	$\sigma(s_1) = s_1 + \frac{1}{k+1}$	

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

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$$\sigma(s_1) = s_1 + f_1 \qquad f_1 \in \mathbb{K}(k)[p_1, p_1^{-1}] \dots [p_e, p_e^{-1}][x]$$

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$$\vdots$$

CONSTRUCT a $R\Pi\Sigma^*$-ring $(\mathbb{A},\sigma)$ for $f(k)$: (Karr81,CS14,CS16)

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

$$\boxed{\mathbb{A} := \mathbb{K}(k)[p_1,p_1^{-1}][p_2,p_2^{-1}]\dots[p_e,p_e^{-1}][x][s_1][s_2][s_3]\dots}$$

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

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

hypergeometric products $\leftrightarrow$

$$\sigma(p_1)=a_1\,p_1 \qquad a_1\in\mathbb{K}(k)^*$$
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α is a primitive λth root of unity $\quad \alpha^{\mathbf{k}} \leftrightarrow$

$$\sigma(\mathbf{x})=\alpha\,\mathbf{x} \qquad \mathbf{x}^{\lambda}=\mathbf{1}$$

(nested) sum $\leftrightarrow$

$$\sigma(s_1)=s_1+f_1 \qquad f_1\in\mathbb{K}(k)[p_1,p_1^{-1}]\dots[p_e,p_e^{-1}][x]$$
$$\sigma(s_2)=s_2+f_2 \qquad f_2\in\mathbb{K}(k)[p_1,p_1^{-1}]\dots[p_e,p_e^{-1}][x][s_1]$$
$$\sigma(s_3)=s_3+f_3 \qquad f_3\in\mathbb{K}(k)[p_1,p_1^{-1}]\dots[p_e,p_e^{-1}][x][s_1][s_2]$$
$$\vdots$$

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

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α is a primitive λth root of unity α^k

(nested) su ... $e, p_e^{-1}][x]$

... $e, p_e^{-1}][x][s_1]$

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

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

$$\sigma(s_3) = s_3 + f_3 \qquad f_3 \in \mathbb{K}(k)[p_1, p_1^{-1}] \dots [p_e, p_e^{-1}][x][s_1][s_2]$$

$$\vdots$$

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

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

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

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

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

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

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

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

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

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

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

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Degree bound: COMPUTE $b \geq 0$: $b = 2$

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

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

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

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

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

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

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

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

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

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

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coeff. comp.

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

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

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coeff. comp.

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

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

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

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

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coeff. comp.

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

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

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

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

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

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coeff. comp.

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

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

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

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.

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

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

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

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

g=hk-k

coeff. comp.

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

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

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

coeff. comp.

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

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

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

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

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 $(\mathbb{A}, \sigma)$ 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 $(\mathbb{A},\sigma)$ with $f\in\mathbb{A}$.

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

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

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1. FIND an appropriate $R\Pi\Sigma^*$-ring $(\mathbb{A}, \sigma)$ 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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$$= \frac{a^2+4a+5}{10(a^2+2a+2)} S_1(a) - \frac{(a-1)(a+1)}{5(a^2+2a+2)} S_3(a) - \frac{2}{5} \sum_{k=1}^{a} \frac{1}{k^2}$$

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appropriate = sum representations with optimal nesting depth

Example:

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

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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

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Example:

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Example:

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

Simplification of nested product-sum expressions

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

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

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

- such that

$A(\lambda) = B(\lambda)$ for all $\lambda \in \mathbb{N}$ with $\lambda \geq \delta$
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- 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)

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

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

$$\mathbb{A} := \mathbb{K}(k)[p_1,p_1^{-1}][p_2,p_2^{-1}]\dots[p_e,p_e^{-1}][x][s_1][s_2][s_3]\dots$$

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

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

hypergeometric products $\leftrightarrow$

$$\sigma(p_1)=a_1\,p_1 \qquad a_1\in\mathbb{K}(k)^*$$
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$$\sigma(p_e)=a_ep_e \qquad a_e\in\mathbb{K}(k)[p_1,p_1^{-1}]\dots[p_{e-1},p_{e-1}^{-1}]^*$$

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$$\sigma(\mathbf{x})=\alpha\,\mathbf{x} \qquad \mathbf{x}^{\lambda}=\mathbf{1}$$

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Theorem. The following statements are equivalent:

1. $\mathrm{const}_\sigma \mathbb{A} = \mathbb{K}$.

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CS, A Difference Ring Theory for Symbolic Summation. J. Symb. Comput. 72, pp. 82-127. 2016.
CS, Summation Theory II: Characterizations of $R\Pi\Sigma$-extensions. To appear in J. Symb. Comput., pp. 1-55. 2016.

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Note: Similar results have been worked out in the Galois theory of difference equations (van der Put/Singer, 1997)

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Note: Works also for the q-rational, multi-basic and mixed case.

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hypergeometric products $\leftrightarrow$

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\sigma(p_1) &= a_1\,p_1 & a_1 &\in \mathbb{K}(k)^*\\
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CONSTRUCT a $R\Pi\Sigma^*$-ring $(\mathbb{A}, \sigma)$ for $A(k)$: (Karr81,CS14,CS16)

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

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We get $a \in \mathbb{A}$ plus
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$$\tau(a) = \langle A(\nu) \rangle_{\nu \geq 0}$$

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Reinterpreting a in terms of these nested sums and products yields $B(k)$

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$$\tau(a)=\langle A(\nu)\rangle_{\nu\geq 0}$$

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Simplification of nested product-sum expressions

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

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

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Application 1: the expression $B(k)$ is usually much smaller

Simplification of nested product-sum expressions

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Application 1: the expression $B(k)$ is usually much smaller

Application 2: We solve the zero-recognition problem.

$A(k)$ evaluates to 0 from a certain point on $\quad\Leftrightarrow\quad B(k) = 0$

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–)

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

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

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

Zeilberger's creative telescoping paradigm

GIVEN

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

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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:

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

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

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

Zeilberger's creative telescoping paradigm

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 $n \geq 0$.

Summing this equation over k from 1 to a gives:

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

$$\lim_{a\to\infty} \,||\qquad\qquad\qquad\qquad ||$$

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

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.

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

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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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.

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

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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]= $$-n\text{SUM}[n] + (1+n)(2+n)\text{SUM}[n+1] == \frac{(a+1)(S[1,a]+S[1,n]-S[1,a+n])}{(n+1)^2(a+n+2)n!} + \frac{a(a+1)}{(n+1)^3(a+n+1)(a+n+2)n!}$$

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

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

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Solve a recurrence

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

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

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

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

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

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

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

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

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Solve a recurrence

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

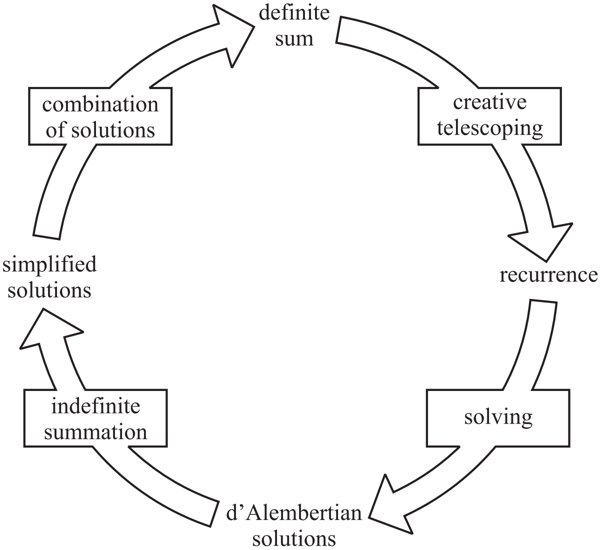
Out[5]= $$\{\{0, \frac{1}{n(n+1)}\}, \{1, \frac{S[1,n]^2 + \sum_{i=1}^{n} \frac{1}{i^2}}{2n(n+1)}\}\}$$

Combine the solutions

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

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

Sigma's summation spiral



Example

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:

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

Integral representation:

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

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Asymptotic expansion:

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

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

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

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

- Generalized algorithms for nested binomial sums

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

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**[

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

The full machinery:

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

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EvaluateMultiSums by Carsten Schneider © RISC-Linz

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

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

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

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

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

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

$60s <$ in a jiffy

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

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

$60s <$ in a jiffy

$=0.999222...$

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

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

Produce variations:

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

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

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

Produce variations:

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

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

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

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

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

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

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

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

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

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

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

Produce variations:

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

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

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

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

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

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

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

Produce variations:

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

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

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

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

Next

Example 2: Super-congruences

(S. Ahlgren, E. Mortenson, R. Osburn, Sigma)

Sigma's contribution to harmonic number congruences

- S. Ahlgren (2001):

$$\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}}{j}^2 \binom{j+\frac{p-1}{2}}{j} \left(H_{j+\frac{p-1}{2}} - H_{\frac{p-1}{2}}\right) \equiv 0 \mod p$$

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- E. Mortenson (2003):

$$\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}}{j}^2 \binom{j+\frac{p-1}{2}}{j} \left(1+3jH_{j+\frac{p-1}{2}} - 3jH_j\right) \equiv 0 \mod p$$

$$\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}}{j} \binom{j+\frac{p-1}{2}}{j} \left(1+2jH_{j+\frac{p-1}{2}} - 2jH_j\right) \equiv 0 \mod p$$

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- S. Ahlgren (2001):

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$$\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}}{j}^2 \binom{j+\frac{p-1}{2}}{j} (1 + 3jH_{j+\frac{p-1}{2}} - 3jH_j) \equiv 0 \mod p$$

$$\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}}{j} \binom{j+\frac{p-1}{2}}{j} (1 + 2jH_{j+\frac{p-1}{2}} - 2jH_j) \equiv 0 \mod p$$

- R. Osburn:

$$p^2\, E_2(p) + p\, E_1(p) + p^0 E_0(p) \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

For a prime $p > 2$,

$$p^2 E_2(p)$$

$$+pE_1(p)$$

$$+p^0 E_0(p) \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

For a prime $p > 2$,

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$$+p^0 \sum_{j=0}^{\frac{p-1}{2}} \binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

For a prime $p > 2$,

$$p^2 E_2(p)$$

$$+p\Big[\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\big(1+j\big(+H_{j+\frac{p-1}{2}}+H_{-j+\frac{p-1}{2}}-2H_j\big)\big)\Big]$$

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For a prime $p > 2$,

$$p^2\Big[\sum_{j=1}^{\frac{p-3}{2}}\Big(\frac{(-1)^j}{\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}}$$

$$+\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\Big(1+4j\big(H_{j+\frac{p-1}{2}}-H_j\big)$$

$$+j^2\Big(2\big(H_{j+\frac{p-1}{2}}-H_j\big)^2+H_j^{(2)}-H_{j+\frac{p-1}{2}}^{(2)}\Big)\Big)\Big]$$

$$+p\Big[\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\Big(1+j\big(+H_{j+\frac{p-1}{2}}+H_{-j+\frac{p-1}{2}}-2H_j\big)\Big)\Big]$$

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$$+j^2\Big(2\big(H_{j+\frac{p-1}{2}}-H_j\big)^2+H_j^{(2)}-H_{j+\frac{p-1}{2}}^{(2)}\Big)\Big)\Big]$$

$$+p\Big[\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\Big(1+j\big(+H_{j+\frac{p-1}{2}}+H_{-j+\frac{p-1}{2}}-2H_j\big)\Big)\Big]$$

$$+p^0\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

$$\sum_{j=1}^{\frac{p-3}{2}} \Big(\frac{(-1)^j}{\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}}$$

$$+ \sum_{j=0}^{\frac{p-1}{2}} (-1)^j \binom{\frac{p-1}{2}}{j} \binom{j+\frac{p-1}{2}}{j} \Big(1 + 4j\big(H_{j+\frac{p-1}{2}} - H_j\big)$$

$$+ j^2\Big(2\big(H_{j+\frac{p-1}{2}} - H_j\big)^2 + H_j^{(2)} - H_{j+\frac{p-1}{2}}^{(2)}\Big)\Big)$$

$$\sum_{j=1}^{n-1} \Big(\frac{(-1)^j}{\binom{n}{j}\binom{j+n}{j}}$$

$$+ \sum_{j=0}^{n} (-1)^j \binom{n}{j} \binom{j+n}{j} \Big(1 + 4j\big(H_{j+n} - H_j\big)$$

$$+ j^2\Big(2\big(H_{j+n} - H_j\big)^2 + H_j^{(2)} - H_{j+n}^{(2)}\Big)\Big)$$

$$\sum_{j=1}^{n-1} \Big(\frac{(-1)^j}{\binom{n}{j}\binom{j+n}{j}}$$

$$+\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{j+n}{j}\big(1+4j\big(H_{j+n}-H_j\big)$$

$$+j^2\big(2\big(H_{j+n}-H_j\big)^2+H_j^{(2)}-H_{j+n}^{(2)}\big)\big)$$

$$||$$

summation spiral

$$(-1)^n((n+1)(2n+1)-\binom{2n}{n})$$

$$\sum_{j=1}^{\frac{p-3}{2}} \Big(\frac{(-1)^j}{\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}}$$

$$+ \sum_{j=0}^{\frac{p-1}{2}} (-1)^j \binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j} \big(1 + 4j\big(H_{j+\frac{p-1}{2}} - H_j\big)$$

$$+ j^2\big(2\big(H_{j+\frac{p-1}{2}} - H_j\big)^2 + H_j^{(2)} - H_{j+\frac{p-1}{2}}^{(2)}\big)\big)$$

$$||$$

$$(-1)^{\frac{p-1}{2}}\big(\big(\frac{p-1}{2}+1\big)p - \binom{p-1}{\frac{p-1}{2}}\big)$$

For a prime $p > 2$,

$$p^2 \Big[\sum_{j=1}^{\frac{p-3}{2}} \Big(\frac{(-1)^j}{\binom{\frac{p-1}{2}}{j} \binom{j+\frac{p-1}{2}}{j}}$$

$$+ \sum_{j=0}^{\frac{p-1}{2}} (-1)^j \binom{\frac{p-1}{2}}{j} \binom{j+\frac{p-1}{2}}{j} \Big(1 + 4j\big(H_{j+\frac{p-1}{2}} - H_j\big)$$

$$+ j^2 \Big(2\big(H_{j+\frac{p-1}{2}} - H_j\big)^2 + H_j^{(2)} - H_{j+\frac{p-1}{2}}^{(2)}\Big)\Big) \Big]$$

$$+ p \Big[\sum_{j=0}^{\frac{p-1}{2}} (-1)^j \binom{\frac{p-1}{2}}{j} \binom{j+\frac{p-1}{2}}{j} \Big(1 + j\big(+ H_{j+\frac{p-1}{2}} + H_{-j+\frac{p-1}{2}} - 2H_j\big)\Big) \Big]$$

$$+ p^0 \sum_{j=0}^{\frac{p-1}{2}} \binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

For a prime $p > 2$,

$$
\begin{aligned}
&p^2\Big[\\
&\qquad (-1)^{\frac{p-1}{2}}\left(\left(\tfrac{p-1}{2}+1\right)p-\binom{p-1}{\frac{p-1}{2}}\right) \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\Big] \\
&+p\Big[\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\left(1+j\left(+H_{j+\frac{p-1}{2}}+H_{-j+\frac{p-1}{2}}-2H_j\right)\right)\Big] \\
&+p^0\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^2 16^{-j} \;\equiv\; (-1)^{\frac{p-1}{2}} \quad \mod p^3
\end{aligned}
$$

For a prime $p > 2$,

$$p^2\Big[$$

$$-(-1)^{\frac{p-1}{2}}\binom{p-1}{\frac{p-1}{2}}$$

$$\Big]$$

$$+p\Big[\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\big(1+j\big(+H_{j+\frac{p-1}{2}}+H_{-j+\frac{p-1}{2}}-2H_j\big)\big)\Big]$$

$$+p^0\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

For a prime $p > 2$,

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$$\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\big(1+j\big(-2Hj+H_{j+\frac{p-1}{2}}+H_{-j+\frac{p-1}{2}}\big)\big)$$

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{j+n}{j}\big(1+j\big(-2Hj+H_{j+n}+H_{-j+n}\big)\big)$$

$$\sum_{j=0}^{n}(-1)^j\binom{n}{j}\binom{j+n}{j}\big(1+j\big(-2Hj+H_{j+n}+H_{-j+n}\big)\big)$$

$$||$$

summation spiral

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

$$\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\big(1+j\big(-2Hj+H_{j+\frac{p-1}{2}}+H_{-j+\frac{p-1}{2}}\big)\big)$$

$$||$$

$$-\frac{3}{2}(-1)^{\frac{p-1}{2}}\Big(\frac{p^2}{4}-\frac{1}{4}\Big)\sum_{j=1}^{\frac{p-1}{2}}\frac{\binom{2j}{j}}{j}+(-1)^{\frac{p-1}{2}}p\binom{p-1}{\frac{p-1}{2}}$$

For a prime $p > 2$,

$$p^2\Big[$$

$$-(-1)^{\frac{p-1}{2}}\binom{p-1}{\frac{p-1}{2}}$$

$$\Big]$$

$$+p\Big[\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\big(1+j\big(+H_{j+\frac{p-1}{2}}+H_{-j+\frac{p-1}{2}}-2H_j\big)\big)\Big]$$

$$+p^0\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

For a prime $p > 2$,

$$p^2\Big[$$

$$-(-1)^{\frac{p-1}{2}}\binom{p-1}{\frac{p-1}{2}}$$

$$\Big]$$

$$+p\Big[-\frac{3}{2}(-1)^{\frac{p-1}{2}}\Big(\frac{p^2}{4}-\frac{1}{4}\Big)\sum_{j=1}^{\frac{p-1}{2}}\frac{\binom{2j}{j}}{j}+(-1)^{\frac{p-1}{2}}p\binom{p-1}{\frac{p-1}{2}}\Big]$$

$$+p^0\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

For a prime $p > 2$,

$$p^2\Big[\qquad 0 \qquad \Big]$$

$$+p\Big[-\frac{3}{2}(-1)^{\frac{p-1}{2}}\Big(\frac{p^2}{4}-\frac{1}{4}\Big)\sum_{j=1}^{\frac{p-1}{2}}\frac{\binom{2j}{j}}{j}\Big]$$

$$+p^0\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

For a prime $p > 2$,

$$p^2\Big[\qquad\qquad 0 \qquad\qquad \Big]$$

$$+p\Big[\frac{3}{8}(-1)^{\frac{p-1}{2}}\sum_{j=1}^{\frac{p-1}{2}}\frac{\binom{2j}{j}}{j}\Big]$$

$$+p^0\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

For a prime $p > 2$,

$$p^2\Big[\sum_{j=1}^{\frac{p-3}{2}}\Big(\frac{(-1)^j}{\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}}$$

$$+\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\Big(1+4j\big(H_{j+\frac{p-1}{2}}-H_j\big)$$

$$+j^2\Big(2\big(H_{j+\frac{p-1}{2}}-H_j\big)^2+H_j^{(2)}-H_{j+\frac{p-1}{2}}^{(2)}\Big)\Big)\Big]$$

$$+p\Big[\sum_{j=0}^{\frac{p-1}{2}}(-1)^j\binom{\frac{p-1}{2}}{j}\binom{j+\frac{p-1}{2}}{j}\Big(1+j\big(+H_{j+\frac{p-1}{2}}+H_{-j+\frac{p-1}{2}}-2H_j\big)\Big)\Big]$$

$$+p^0\sum_{j=0}^{\frac{p-1}{2}}\binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

Sigma's contribution to harmonic number congruences

- S. Ahlgren (2001):

$$\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}}{j}^2 \binom{j+\frac{p-1}{2}}{j} (H_{j+\frac{p-1}{2}} - H_{\frac{p-1}{2}}) \equiv 0 \mod p$$

- E. Mortenson (2003):

$$\sum_{j=0}^{\frac{p-1}{2}} \binom{\frac{p-1}{2}}{j}^2 \binom{j+\frac{p-1}{2}}{j} (1 + 3jH_{j+\frac{p-1}{2}} - 3jH_j) \equiv 0 \mod p$$

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- R. Osburn/CS (2008):

$$p\,\frac{3}{8}(-1)^{\frac{p-1}{2}} \sum_{j=1}^{\frac{p-1}{2}} \frac{\binom{2j}{j}}{j} + \sum_{j=0}^{\frac{p-1}{2}} \binom{2j}{j}^2 16^{-j} \equiv (-1)^{\frac{p-1}{2}} \mod p^3$$

Example 3: Feynman integrals

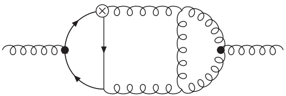
joint work (RISC–DESY) with

J. Ablinger, A. Behring, I. Bierenbaum, J. Blümlein, A. Hasselhuhn,

A. de Freitas, A. von Manteuffel, C.G. Raab, M. Round, S. Klein, F. Wißbrock

Evaluation of Feynman diagrams

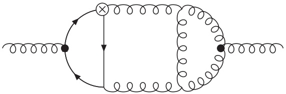
(long term project with J. Blümlein, Deutsches Elektronen–Synchrotron)



Behavior of particles

Evaluation of Feynman diagrams

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



Behavior of particles

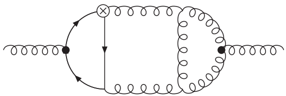
$\longrightarrow$

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

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

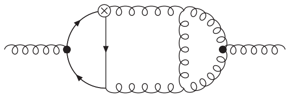
DESY

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

multi sums

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

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

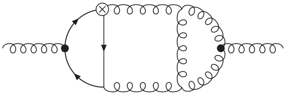
multi sums

symbolic summation

expressions in terms of special functions

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

symbolic summation

expressions in terms of special functions

processable by physicists

Evaluations required for the LHC experiment at CERN

A warm-up example: simplify

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

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

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

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

Simple sum

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

$$||$$

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

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

$$||$$

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

$$||$$

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

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

$$||$$

$$\sum_{j=0}^{n-2}\boxed{\begin{aligned}&\sum_{r=0}^{j+1}\binom{j+1}{r}\Big(\frac{(-1)^r(-j+n-2)!r!}{(n+1)(-j+n+r-1)(-j+n+r)!}+\\&\qquad\frac{(-1)^{n+r}(j+1)!(-j+n-2)!(-j+n-1)_r r!}{(n-1)n(n+1)(-j+n+r)!(-j-1)_r(2-n)_j}\Big)\end{aligned}}$$

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

$$||$$

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

$$||$$

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

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

$$||$$

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

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

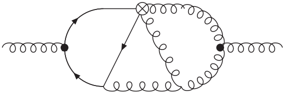
$$||$$

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

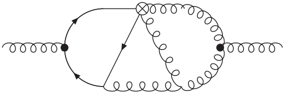
$$||$$

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

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



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



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

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**

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

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

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

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

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

$F_0(n) =$

$\frac{7}{12}S_1(n)^4 + \frac{(17n+5)S_1(n)^3}{[illegible](n+1)} + \big(\frac{35n^2-2n-5}{2n^2(n+1)^2} + \frac{13S_2(n)}{2} + \frac{5(-1)^n}{2n^2}\big)S_1(n)^2$

$+ \big($ [illegible] $1)^n(2n+1)}{n(n+1)} - \frac{13}{n}\big)S_2(n) + \big(\frac{29}{3} - (-1)^n\big)S_3(n)$

$+ \big(2 +$ [illegible] $- 28S_{-2,1}(n) + \frac{20(-1)^n}{n^2(n+1)}\big)$ [illegible] $\big)S_2(n)^2$

$- 2(-1)^nS_{-2}(n)^2 + S_{-3}(n)\big(\frac{2(3n-5)}{n(n+1)} + \big(26 + 4($ [illegible] $\big)$

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

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

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

$+ \big(-\frac{2(-1)^n(9n+5)}{n(n+1)} - \frac{2}{n}\big)S_{2,1}(n) + \big(20 + 2(-1)^n\big)S_{2,-2}(n) + \big(-17 + 13(-1)^n\big)S_{3,1}(n)$

$- \frac{8(-1)^n(2n+1) + 4(9n+1)}{n(n+1)}S_{-2,1}(n) - \big(24 + 4(-1)^n\big)S_{-3,1}(n) + \big(3 - 5(-1)^n\big)S_{2,1,1}(n)$

$+ 32S_{-2,1,1}(n) + \left(\frac{3}{2}S_1(n)^2 - \frac{3S_1(n)}{n} + \frac{3}{2}(-1)^nS_{-2}(n)\right)\zeta(2)$

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

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

$F_0(n)$ =

$$\frac{7}{12}S_1(n)^4 + \frac{(17n+5)S_1(n)^3}{\ldots} + \Big(\frac{35n^2-2n-5}{2n^2(n+1)^2} + \frac{13S_2(n)}{2} + \frac{5(-1)^n}{2n^2}\Big)S_1(n)^2$$

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

$$+ \Big(2 + \ldots - 28S_{-2,1}(n) + \frac{20(-1)^n}{n^2(n+1)}\Big) \ldots \Big) S_2(n)^2$$

$$- 2(-1)^n S_{-2}(n)^2 + S_{-3}(n)\Big(\frac{2(3n-5)}{n(n+1)} + \big(26 + 4(\ldots \Big)$$

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

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

$$+ \Big(\frac{(-1) \ldots}{n(\ldots} \ldots n) + \big(-6 + 5(-1)^n\big)S_{-4}(n)$$

$$+ \Big(- \frac{2(\ldots}{\ldots} \ldots S_{2,-2}(n) + \big(-17 + 13(-1)^n\big)S_{3,1}(n)$$

$$- \frac{8(-1)^{\ldots}}{n(n+1)} S_{-2,1}(n) - \big(24 + 4(-1)^n\big)S_{-3,1}(n) + \big(3 - 5(-1)^n\big)S_{2,1,1}(n)$$

$$+ 32S_{-2,1,1}(n) + \left(\frac{3}{2}S_1(n)^2 - \frac{3S_1(n)}{n} + \frac{3}{2}(-1)^n S_{-2}(n)\right)\zeta(2)$$

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

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

So far derived results (in 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.
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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].
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5. J. Ablinger, ... Wissbrock. The Transition M... ...s B 882, pp. 263-288. 20...
6. J. Ablinger, ... Operator Matrix Elements by ...
7. J. Ablinger, ... the $O(\alpha_s^3 T_F^2)$ Contribution...
8. J. Ablinger, A... 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.
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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

More details:

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Calculations rely heavily on:

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Calculations rely heavily on:

- advanced difference ring and special function algorithms
- efficient implementations for large expressions
- reliable software based on proof certificates