

AMS Special Session on
"Applications of Computer Algebra in Enumerative and Algebraic
Combinatorics"

Multi-Summation in Difference Fields

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Starting point:
bonus problem 6.69 in “Concrete Mathematics”

FIND a closed form for

$$\sum_{k=1}^n k^2 H_{n+k} = ?$$

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

D.E. Knuth:

“It would be nice to automate the derivation of formulas such as this.”

Telescoping

GIVEN $f(k) = k^2 H_{n+k}$.

FIND $g(k)$:

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

Telescoping

GIVEN $f(k) = k^2 H_{n+k}$.

FIND $g(k)$:

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

Sigma computes

$$g(k) = \frac{1}{36} (k(-4k^2 + (6n+3)k - 12n(n+1) + 1) + 6(2k^3 - 3k^2 + k + n(n+1)(2n+1))H_{k+n}).$$

Telescoping

GIVEN $f(k) = k^2 H_{n+k}$.

FIND $g(k)$:

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

Summing the telescoping equation over k from 1 to n gives

$$\sum_{k=1}^n k^2 H_{n+k} = g(n+1) - g(1)$$

$$= -\frac{1}{36}n(n+1)(10n+6(2n+1)H_n - 12(2n+1)H_{2n} - 1).$$

Telescoping

GIVEN $f(k) = k^2 H_{n+k}$.

FIND $g(k)$:

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

A difference field for the **summand**:

Take the rational function field

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

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

Karr 1981

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

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

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

$$S k = k + 1,$$

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

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

Telescoping

GIVEN $f(k) = k^2 H_{n+k}$.

FIND $g(k)$:

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

↓

GIVEN $f := k^2 h \in \mathbb{F}$.

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

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

Telescoping

GIVEN $f(k) = k^2 H_{n+k}$.

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↓ Sigma

$$g = \frac{1}{36} (k(-4k^2 + (6n+3)k - 12n(n+1) + 1) + 6(2k^3 - 3k^2 + k + n(n+1)(2n+1))h)$$

Telescoping

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FIND $g(k)$:

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$$g = \frac{1}{36} (k(-4k^2 + (6n+3)k - 12n(n+1) + 1) + 6(2k^3 - 3k^2 + k + n(n+1)(2n+1)))h$$

↑
 $h \equiv H_{n+k}$

Example 1: A quadruple sum

A challenging email:

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:

$$\sum_{j,k=1}^{\infty} \frac{H_j(H_{k+1}-1)}{jk(k+1)(j+k)}; \quad H_j := \sum_{i=1}^j \frac{1}{i}.$$

Simplify:

$$\sum_{k=1}^{\infty} \frac{H_{k+1} - 1}{k(k+1)} \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)}.$$

$$\sum_{j=1}^a \frac{H_j}{j(j+k)} = \text{FIND}$$

Simplify:

$$\sum_{k=1}^{\infty} \frac{H_{k+1} - 1}{k(k+1)} \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)}.$$

$$\sum_{j=1}^a \frac{H_j}{j(j+k)} = \frac{kH_k^2 - 2H_k + kH_k^{(2)} + 2kH_a^{(2)}}{2k^2}$$

$$- \underbrace{\frac{(kH_a - 1)}{k^2} \sum_{i=1}^k \frac{1}{a+i} - \frac{1}{k} \sum_{i=1}^k \frac{1}{i} \sum_{j=1}^i \frac{1}{a+j}}_{\text{Limits}}$$

Simplify:

$$\sum_{k=1}^{\infty} \frac{H_{k+1} - 1}{k(k+1)} \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)}.$$

$$\sum_{j=1}^{\infty} \frac{H_j}{j(j+k)} = \frac{kH_k^2 - 2H_k + kH_k^{(2)} + 2k\zeta(2)}{2k^2}$$

Simplify:

$$\sum_{k=1}^{\infty} \frac{H_{k+1} - 1}{k(k+1)} \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)}.$$

$$\sum_{k=1}^b \frac{H_{k+1} - 1}{k(k+1)} \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)} = \sum_{k=1}^b \frac{H_{k+1} - 1}{k(k+1)} \frac{kH_k^2 - 2H_k + kH_k^{(2)} + 2k\zeta(2)}{2k^2}$$

= Sigma

Simplify:

$$\sum_{k=1}^{\infty} \frac{H_{k+1} - 1}{k(k+1)} \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)}.$$

$$\begin{aligned} \sum_{k=1}^b \frac{H_{k+1} - 1}{k(k+1)} \sum_{j=1}^{\infty} \frac{H_j}{j(j+k)} &= \sum_{k=1}^b \frac{H_{k+1} - 1}{k(k+1)} \frac{kH_k^2 - 2H_k + kH_k^{(2)} + 2k\zeta(2)}{2k^2} \\ &= \frac{1}{2(b+1)^2} \left(6H_b + 4bH_b + 4H_b^2 + 3bH_b^2 + H_b^3 + bH_b^3 - 6b\zeta(2) \right. \\ &\quad \left. + 2H_b\zeta(2) + 2bH_b\zeta(2) - 2H_b^{(2)} - 7bH_b^{(2)} + H_bH_b^{(2)} + bH_bH_b^{(2)} \right) \\ &\quad - \frac{2b^2}{(b+1)^2} \left(\zeta(2) + H_b^{(2)} \right) \\ &\quad + (\zeta(2) - 1) \sum_{i=1}^b \frac{H_i}{i^2} - \sum_{i=1}^b \frac{H_i^2}{i^3} + \frac{1}{2} \sum_{i=1}^b \frac{H_i^3}{i^2} + \frac{1}{2} \sum_{i=1}^b \frac{H_i H_i^{(2)}}{i^2} \end{aligned}$$

ζ -relations

This gives

$$\begin{aligned} S &= \sum_{j,k=1}^{\infty} \frac{H_j(H_{k+1} - 1)}{jk(k+1)(j+k)} \\ &= -4\zeta(2) + (\zeta(2) - 1) \sum_{i=1}^{\infty} \frac{H_i}{i^2} - \sum_{i=1}^{\infty} \frac{H_i^2}{i^3} + \frac{1}{2} \sum_{i=1}^{\infty} \frac{H_i^3}{i^2} + \frac{1}{2} \sum_{i=1}^{\infty} \frac{H_i H_i^{(2)}}{i^2}. \end{aligned}$$

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 &= -4\zeta(2) + (\zeta(2) - 1) \sum_{i=1}^{\infty} \frac{H_i}{i^2} - \sum_{i=1}^{\infty} \frac{H_i^2}{i^3} + \frac{1}{2} \sum_{i=1}^{\infty} \frac{H_i^3}{i^2} + \frac{1}{2} \sum_{i=1}^{\infty} \frac{H_i H_i^{(2)}}{i^2}.
 \end{aligned}$$

E.g., in J.M. Borwein, Girgensohn. Evaluation of triple Euler sums, 1996.

Flajolet, Salvy. Euler sums and contour integral representations, 1998.

we find

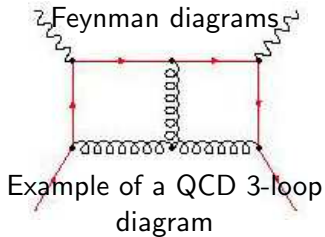
$$\begin{aligned}
 \sum_{i=1}^{\infty} \frac{H_i}{i^2} &= 2\zeta(3), & \sum_{i=1}^{\infty} \frac{H_i^2}{i^3} &= -\zeta(2)\zeta(3) + \frac{7}{2}\zeta(5), \\
 \sum_{i=1}^{\infty} \frac{H_i^3}{i^2} &= \zeta(2)\zeta(3) + 10\zeta(5), & \sum_{i=1}^{\infty} \frac{H_i H_i^{(2)}}{i^2} &= \zeta(2)\zeta(3) + \zeta(5).
 \end{aligned}$$

Theorem (Sigma 2005).

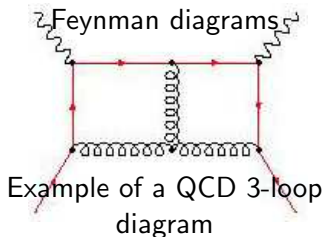
$$S = \sum_{j,k=1}^{\infty} \frac{H_j(H_{k+1} - 1)}{jk(k+1)(j+k)}$$
$$= -4\zeta(2) - 2\zeta(3) + 4\zeta(2)\zeta(3) + 2\zeta(5) = 0.999222\dots$$

Example 2: Evaluation of Feynman integrals

Feynman diagrams



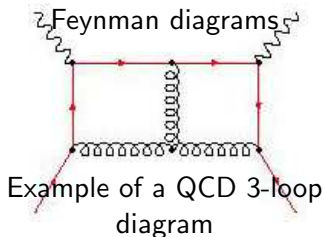
Example 2: Evaluation of Feynman integrals



$$\int \Phi(x) dx$$

Task: Evaluation of Feynman integrals

Example 2: Evaluation of Feynman integrals



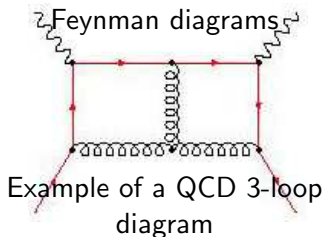
$$\longrightarrow \int \Phi(x) dx$$

Task: Evaluation of Feynman integrals

Reduction
(J. Blümlein; DESY)

multi-sums (similar to Exp. 1)/
recurrences

Example 2: Evaluation of Feynman integrals



$$\longrightarrow \int \Phi(x) dx$$

Task: Evaluation of Feynman integrals

Reduction
(J. Blümlein; DESY)



Simplified expressions/
solutions

Sigma multi-sums (similar to Exp. 1)/
recurrences



In the non-singlet (3-loop) case ~ 360 diagrams contribute. The integrals are of the form:

$$F(n, \varepsilon) = \int_0^1 dx_1 \dots \int_0^1 dx_7 \sum_{i=1}^K \frac{p_i(x_1, x_2, \dots, x_7)^{n+\dots+r_i\varepsilon+\dots}}{q_i(x_1, x_2, \dots, x_7)^{\dots+s_i\varepsilon+\dots}}$$

where $K \in \mathbb{N}$, $r_i, s_i \in \mathbb{Q}$, and p_i, q_i are polynomials in x_1, \dots, x_7 .

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

The **3-loop anomalous dimensions** can be derived from the single pole part of $F(n, \varepsilon)$. The other poles are needed for the **renormalization**.

Vermaseren, Moch: 3-5 CPU years (2004)

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 \end{aligned}$$

↓

Initial values $F_{-1}(i)$, $i = 1, \dots, 450$

↓ Recurrence finder (M. Kauers)

$$a_0(n)F_{-1}(n) + a_1(n)F_{-1}(n+1) + \dots + a_7(n)F_{-1}(n+7) = 0$$

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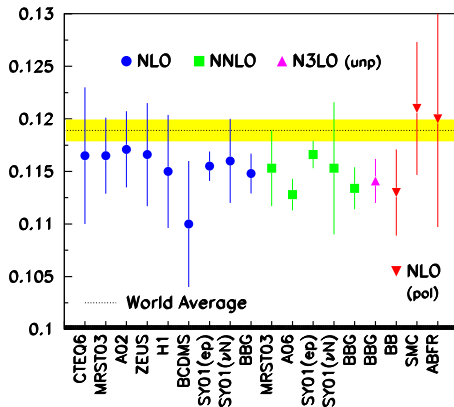
$$a_0(n)F_{-1}(n) + a_1(n)F_{-1}(n+1) + \dots + a_7(n)F_{-1}(n+7) = 0$$

↓

Sigma

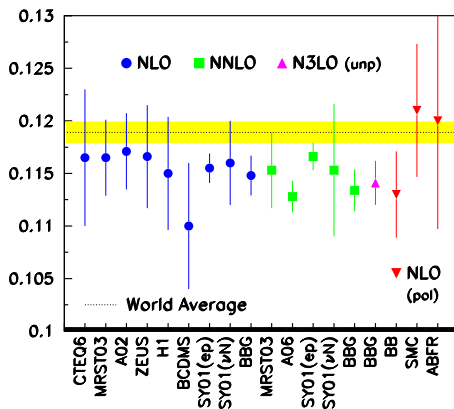
CLOSED FORM

Improvement of the measurement of the coupling constant of the strong force







2-loop result → **3-loop result**

Improvement of the measurement of the coupling constant of the strong force



2-loop result → 3-loop result → 4-loop challenge

Appendix

- ▶ Integration 
- ▶ $\Pi\Sigma$ -fields 
- ▶ Padé approximation 
- ▶ Creative telescoping 

Sigma's algorithmic summation paradigms

GIVEN a definite sum

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

FIND a recurrence for $S(n)$ in n (Z 's creative extension of telescoping).

Sigma's algorithmic summation paradigms

GIVEN a **definite** sum

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

FIND a **recurrence** for $S(n)$ in n (Z 's creative extension of telescoping).



GIVEN a recurrence

$$a_d(n)S(n+d) + \cdots + a_1(n)S(n+1) + a_0(n)S(n) = h(n).$$

FIND **all solutions** in $\Pi\Sigma$ -extensions (d'Alembertian solutions).

Sigma's algorithmic summation paradigms

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FIND all solutions in $\Pi\Sigma$ -extensions (d'Alembertian solutions).



FIND an alternative representation:

$$S(n) = \text{combined solutions.}$$

$\Pi\Sigma$ -Fields

[▶ Telescoping](#)[▶ Appendix](#)

- ▶ Let $\mathbb{K}(t_1, t_2, \dots, t_e)$ be a rational function field.
- ▶ Let σ be a field automorphism of $\mathbb{K}(t_1) \dots (t_e)$ with

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

$\Pi\Sigma$ -Fields

▸ Telescoping

▸ Appendix

- ▶ Let $\mathbb{K}(t_1, t_2, \dots, t_e)$ be a rational function field.
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$$\begin{aligned}\sigma(c) &= c \quad \forall c \in \mathbb{K} \\ \sigma(t_1) &= \alpha_1 t_1 + \beta_1, \quad \alpha_1, \beta_1 \in \mathbb{K}\end{aligned}$$

$\Pi\Sigma$ -Fields

▸ Telescoping

▸ Appendix

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$\Pi\Sigma$ -Fields

▸ Telescoping

▸ Appendix

- ▶ Let $\mathbb{K}(t_1, t_2, \dots, t_e)$ be a rational function field.
- ▶ Let σ be a field automorphism of $\mathbb{K}(t_1) \dots (t_e)$ with

$$\begin{aligned}\sigma(c) &= c & \forall c \in \mathbb{K} \\ \sigma(t_1) &= \alpha_1 t_1 + \beta_1, & \alpha_1, \beta_1 \in \mathbb{K} \\ \sigma(t_2) &= \alpha_2 t_2 + \beta_2, & \alpha_2, \beta_2 \in \mathbb{K}(t_1) \\ & \vdots & \\ \sigma(t_e) &= \alpha_e t_e + \beta_e, & \alpha_e, \beta_e \in \mathbb{K}(t_1, \dots, t_{e-1}).\end{aligned}$$

$\Pi\Sigma$ -Fields

▸ Telescoping

▸ Appendix

- ▶ Let $\mathbb{K}(t_1, t_2, \dots, t_e)$ be a **rational function field**.
- ▶ Let σ be a **field automorphism** of $\mathbb{K}(t_1) \dots (t_e)$ with

$$\begin{aligned} \sigma(c) &= c & \forall c \in \mathbb{K} \\ \sigma(t_1) &= \alpha_1 t_1 + \beta_1, & \alpha_1, \beta_1 \in \mathbb{K} \\ \sigma(t_2) &= \alpha_2 t_2 + \beta_2, & \alpha_2, \beta_2 \in \mathbb{K}(t_1) \\ & \vdots & \\ \sigma(t_e) &= \alpha_e t_e + \beta_e, & \alpha_e, \beta_e \in \mathbb{K}(t_1, \dots, t_{e-1}). \end{aligned}$$

- ▶ Then $(\mathbb{K}(t_1, \dots, t_e), \sigma)$ is a **$\Pi\Sigma$ -field** if the set of constants is \mathbb{K} , i.e.,

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

Constructive difference field theory

Summation and Integration

▶ Telescoping

▶ Appendix

Indefinite summation

GIVEN $f(k)$ FIND $g(k)$:

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

 \downarrow

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

Integration

GIVEN $f(x)$ FIND $g(x)$:

$$D_x g(x) = f(x)$$

 \downarrow

$$g(b) - g(a) = \int_a^b f(x) dx$$

Example from quadratic Padé approximation

▶ Appendix

For all $m \geq 0$,

$$\sum_{k=0}^m (-1)^k \binom{m}{k}^3 \left[3(H_{m-k} - H_k)^2 + H_{m-k}^{(2)} + H_k^{(2)} \right] = 0$$

where

$$H_k = \sum_{i=1}^k \frac{1}{i}, \quad H_k^{(2)} = \sum_{i=1}^k \frac{1}{i^2}.$$

Example from quadratic Padé approximation

▶ Appendix

Theorem (Sigma; 2002)

For all $m \geq 0$,

$$\sum_{k=0}^m (-1)^k \binom{m}{k}^3 \left[3(H_{m-k} - H_k)^2 + H_{m-k}^{(2)} + H_k^{(2)} \right] = 0$$

where

$$H_k = \sum_{i=1}^k \frac{1}{i}, \quad H_k^{(2)} = \sum_{i=1}^k \frac{1}{i^2}.$$

Proof.

Sigma

□

Zeilberger's creative telescoping paradigm

▶ Paradigms

▶ Appendix

GIVEN

$$\text{SUM}(m) := \sum_{k=0}^m (-1)^k \binom{m}{k}^3 \underbrace{\left[3(H_{m-k} - H_k)^2 + H_{m-k}^{(2)} + H_k^{(2)} \right]}_{=: f(m, k)}.$$

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

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

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

Zeilberger's creative telescoping paradigm

▶ Paradigms

▶ Appendix

GIVEN

$$\text{SUM}(m) := \sum_{k=0}^m (-1)^k \binom{m}{k}^3 \underbrace{\left[3(H_{m-k} - H_k)^2 + H_{m-k}^{(2)} + H_k^{(2)} \right]}_{=: f(m, k)}.$$

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

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

for all $0 \leq k \leq m$ and all $m \geq 0$.**Sigma:**

$$c_0(m) := 3(3m+2)(3m+4)(3m+8), \quad c_1(m) := 0, \\ c_2(m) := (m+2)^2(3m+8),$$

$$g(m, k) := (-1)^k \binom{m}{k}^3 \frac{p_1(k, m, H_k, H_k^{(2)}, H_{m-k}, H_{m-k}^{(2)})}{(m-k+1)^5 (m-k+2)^5},$$

$$g(m, k+1) := (-1)^k \binom{m}{k}^3 \frac{p_2(k, m, H_k, H_k^{(2)}, H_{m-k}, H_{m-k}^{(2)})}{(m-k+1)^5}.$$

Zeilberger's creative telescoping paradigm

▸ Paradigms

▸ Appendix

GIVEN

$$\text{SUM}(m) := \underbrace{\sum_{k=0}^m (-1)^k \binom{m}{k}^3 \left[3(H_{m-k} - H_k)^2 + H_{m-k}^{(2)} + H_k^{(2)} \right]}_{=: f(m, k)}.$$

GIVEN $c_0(m)$, $c_1(m)$, $c_2(m)$, and $g(m, k)$:

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

for all $0 \leq k \leq m$ and all $m \geq 0$.Summing this equation over k from 0 to m gives:

$$\boxed{g(m, m+1) - g(m, 0)}$$

$$= \boxed{\begin{aligned} &c_0(m) \text{SUM}(m) + \\ &c_1(m) [\text{SUM}(m+1) - f(m+1, m+1)] \\ &c_2(m) [\text{SUM}(m+2) - f(m+2, m+1) - f(m+2, m+2)]. \end{aligned}}$$

Indefinite nested sum expression:

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

Definite nested sum expression:

$$\sum_{k=0}^a \left(\sum_{i=0}^k \binom{n+k}{i} \right)$$