The 4th International Conference on Symbolic and Numerical Scientific Computing (SNSC'08)

Symbolic Summation and its Application in Particle Physics

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Starting point:
bonus problem 6.69 in "Concrete Mathematics"

FIND a closed form for

$$\sum_{k=1}^{n} k^2 \mathsf{H}_{n+k} = \text{?},$$

where $\mathsf{H}_n := \sum_{k=1}^{n} \frac{1}{k}$.

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 $g(k)$:

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

Telescoping

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FIND $g(k)$:

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Sigma computes

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

Telescoping

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

FIND $g(k)$:

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

Summing the telescoping equation over k from 1 to n gives

$$\boxed{\sum_{k=1}^{n} k^2 \mathsf{H}_{n+k}} = \boxed{g(n+1) - g(1)}$$

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

Extensions/Generalizations within the SFB F013

Karr's summation algorithm [1981]
(based on difference fields)

↓ 10 years (SFB F013)

Summation Sigma package [2008]
(efficient algorithms with new extensions/generalizations)

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:
```

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

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:

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

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

$$=\frac{1}{2(b+1)^2}\Big(6H_b+4bH_b+4H_b^2+3bH_b^2+H_b^3+bH_b^3-6b\zeta(2)$$

$$+2H_b\zeta(2)+2bH_b\zeta(2)-2H_b^{(2)}-7bH_b^{(2)}+H_bH_b^{(2)}+bH_bH_b^{(2)}\Big)$$

$$-\frac{2b^2}{(b+1)^2}\Big(\zeta(2)+H_b^{(2)}\Big)$$

$$+(\zeta(2)-1)\sum_{i=1}^{b}\frac{H_i}{i^2}-\sum_{i=1}^{b}\frac{H_i^2}{i^3}+\frac{1}{2}\sum_{i=1}^{b}\frac{H_i^3}{i^2}+\frac{1}{2}\sum_{i=1}^{b}\frac{H_iH_i^{(2)}}{i^2}$$

ζ-relations

This gives

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

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

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

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

we find

$$\sum_{i=1}^{\infty}\frac{H_i}{i^2} = 2\zeta(3), \qquad \sum_{i=1}^{\infty}\frac{H_i^2}{i^3} = -\zeta(2)\zeta(3) + \frac{7}{2}\zeta(5),$$

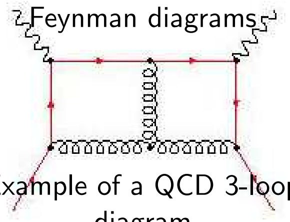
$$\sum_{i=1}^{\infty}\frac{H_i^3}{i^2} = \zeta(2)\zeta(3) + 10\zeta(5), \qquad \sum_{i=1}^{\infty}\frac{H_iH_i^{(2)}}{i^2} = \zeta(2)\zeta(3) + \zeta(5).$$

Theorem (Sigma 2005).

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

$$= -4\zeta(2) - 2\zeta(3) + 4\zeta(2)\zeta(3) + 2\zeta(5) = 0.999222...$$

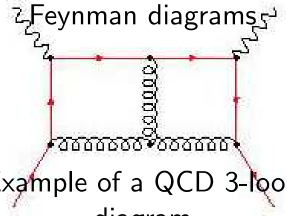
Example 2: Evaluation of Feynman integrals



Example of a QCD 3-loop diagram

Example 2: Evaluation of Feynman integrals

Feynman diagrams



Example of a QCD 3-loop diagram

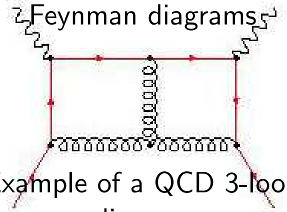
$\longrightarrow$

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

Task: Evaluation of Feynman integrals

Example 2: Evaluation of Feynman integrals

Feynman diagrams



Example of a QCD 3-loop diagram

$\longrightarrow$

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

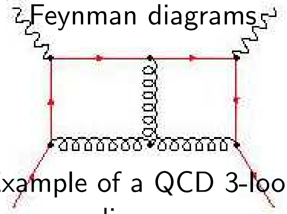
Task: Evaluation of Feynman integrals

$\downarrow$ Reduction (J. Blümlein; DESY)

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

Example 2: Evaluation of Feynman integrals

Feynman diagrams



Example of a QCD 3-loop diagram

⟶

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

Task: Evaluation of Feynman integrals

Reduction
(J. Blümlein; DESY)

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

Sigma ⟵

Simplified expressions/ solutions

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

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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$$\downarrow$$

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

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

$\downarrow$ 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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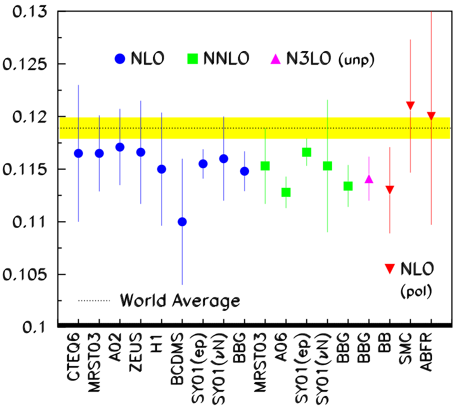
$\downarrow$ Sigma

CLOSED FORM

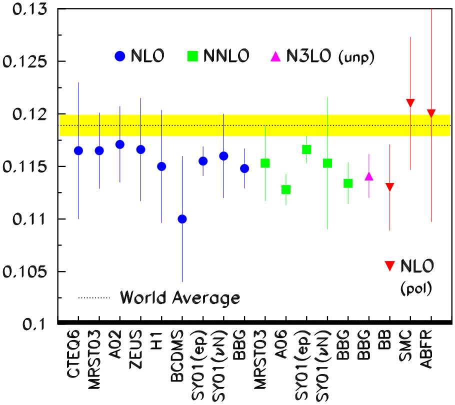
BIG

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



2-loop result $\longrightarrow$ 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

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$$\downarrow$$

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

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↓

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

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

↓

FIND an alternative representation:

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

ΠΣ-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

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$$\sigma(c) = c \qquad \forall c \in \mathbb{K}$$
$$\sigma(t_1) = \alpha_1\, t_1 + \beta_1, \qquad \alpha_1, \beta_1 \in \mathbb{K}$$

$\Pi\Sigma$-Fields

▸ Telescoping ▸ Appendix

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- Let σ be a field automorphism of $\mathbb{K}(t_1)\dots(t_e)$ with

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

$$\sigma(t_1) = \alpha_1\, t_1 + \beta_1, \qquad \alpha_1, \beta_1 \in \mathbb{K}$$

$$\sigma(t_2) = \alpha_2\, t_2 + \beta_2, \qquad \alpha_2, \beta_2 \in \mathbb{K}(t_1)$$

$\Pi\Sigma$-Fields

▸ Telescoping ▸ Appendix

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

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

ΠΣ-Fields

▸ Telescoping ▸ Appendix

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

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

- Then $(\mathbb{K}(t_1, \ldots, t_e), \sigma)$ is a ΠΣ-field if the set of constants is $\mathbb{K}$, i.e.,

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

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 $m \geq 0$*,*

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

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

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

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

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

Sigma:

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

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

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

Zeilberger's creative telescoping paradigm

Paradigms Appendix

GIVEN

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

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

Summing this equation over k from 0 to m gives:

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

$$= \boxed{\begin{array}{l} c_0(m)\,\mathsf{SUM}(m) + \\ c_1(m)\left[\mathsf{SUM}(m+1) - f(m+1,m+1)\right] \\ c_2(m)\left[\mathsf{SUM}(m+2) - f(m+2,m+1) - f(m+2,m+2)\right]. \end{array}}$$

Back

Indefinite nested sum expression:

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

Definite nested sum expression:

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