Trisemestre on Methods of Proof Theory in Mathematics (Seminar Talks)

Max Planck Institute for Mathematics, Bonn

Symbolic Summation and Applications

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Warmup example (bonus problem 6.69 in "Concrete Mathematics")

FIND a closed form for

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

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

Telescoping

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

FIND $g(k)$:

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

for all $1 \leq k \leq n$ and $n \geq 0$.

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Sigma computes

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

Telescoping

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

FIND $g(k)$:

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for all $1 \leq k \leq n$ and $n \geq 0$.

Summing this equation over k from 1 to n gives

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

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

Telescoping

FIND a closed form for

$$\sum_{k=1}^{n} H_k.$$

A difference field for the summand

Consider the rational function field

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

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

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

Telescoping in the given difference field

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

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

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

with

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

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This gives

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

with

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

Hence,

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

▸ Details ▸ General ▸▸ Example 1

telescoping

- GIVEN

$$f(k)\in\mathbb{F}.$$

- FIND $g(k)\in\mathbb{F}$:

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

telescoping

- GIVEN

$$f(k) \in \mathbb{F}.$$

- FIND $g(k) \in \mathbb{F}$:

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

- THEN (with some mild extra conditions)

$$\sum_{k=0}^{n} f(k) = g(n+1) - g(0)$$

Refined telescoping

- GIVEN
$$f(k) \in \mathbb{F}.$$
- FIND $g(k) \in \mathbb{F}$ and $f^*(k)$:
$$\boxed{f(k) = g(k+1) - g(k) + f^*(k)}$$

where $f^*(k)$ is simpler than $f(k)$.

Refined telescoping

- GIVEN

$$f(k)\in\mathbb{F}.$$

- FIND $g(k)\in\mathbb{F}$ and $f^*(k)$:

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

  where $f^*(k)$ is simpler than $f(k)$.

- THEN (with some mild extra conditions)

$$\sum_{k=0}^{n}f(k)=g(n+1)-g(0)+\sum_{k=0}^{n}f^*(k).$$

Simpler w.r.t. the depth

$$\sum_{k=1}^{n} H_k^2 H_k^{(2)} =$$

$$\sum_{k=0}^{a} \left(\sum_{i=0}^{k} \binom{n}{i} \right)^2 =$$

Sigma

$$\sum_{k=1}^{n} \frac{\sum_{j=1}^{k} \frac{\sum_{i=1}^{j} \frac{1}{i}}{j^2}}{k^3} =$$

Simpler w.r.t. the depth

$$\sum_{k=1}^{n} H_k^2 H_k^{(2)} = \frac{1}{3} H_n^{(3)} - \frac{1}{3} H_n^3 + \left((n+1) H_n^{(2)} + 1\right) H_n^2 + (2n+1)\left(1 - H_n\right) H_n^{(2)} - 2H_n$$

$$\sum_{k=0}^{a}\left(\sum_{i=0}^{k}\binom{n}{i}\right)^2 = (n-a)\binom{n}{a}\sum_{i=0}^{a}\binom{n}{i} - \frac{n-2a-2}{2}\left(\sum_{i=0}^{a}\binom{n}{i}\right)^2 - \frac{n}{2}\sum_{i=1}^{a}\binom{n}{i}^2$$

$$\sum_{k=1}^{n}\frac{\sum_{j=1}^{k}\frac{\sum_{i=1}^{j}\frac{1}{i}}{j^2}}{k^3} =$$

$$= H_n^{(3)}\sum_{j=1}^{n}\frac{H_j}{j^2} - \sum_{j=1}^{n}\frac{H_j H_j^{(3)}}{j^2} + \sum_{j=1}^{n}\frac{H_j}{j^5}$$

Simpler w.r.t. the depth

$$\sum_{k=1}^{n} H_k^2 H_k^{(2)} = \tfrac{1}{3} H_n^{(3)} - \tfrac{1}{3} H_n^3 + \left((n+1) H_n^{(2)} + 1\right) H_n^2 + (2n+1)\left(1 - H_n\right) H_n^{(2)} - 2H_n$$

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$$\sum_{k=1}^{n}\frac{\sum_{j=1}^{k}\frac{\sum_{i=1}^{j}\frac{1}{i}}{j^2}}{k^3} = S(3,2,1,n)$$

(Harmonic sums;
alternative representation: Euler-Zagier sums)

$$= H_n^{(3)}\sum_{j=1}^{n}\frac{H_j}{j^2} - \sum_{j=1}^{n}\frac{H_j H_j^{(3)}}{j^2} + \sum_{j=1}^{n}\frac{H_j}{j^5}$$

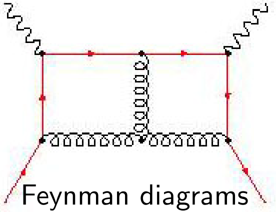
(Euler sums)

Example 1: Particle physics

A. Mitov, S. Moch; *QCD corrections to semi-inclusive hadron production in electron-positron annihilation at two loops*. 2006.

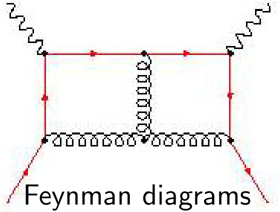
Example 2

Visualization of quantum electrodynamic interaction:



Feynman diagrams

Visualization of quantum electrodynamic interaction:



Feynman diagrams

$$\longrightarrow \quad \int d^D p_1 \dots d^D p_n \frac{1}{(p_1^2)^{v_1} \dots (p_n^2)^{v_n}}$$

GOAL: Evaluation of Feynman integrals

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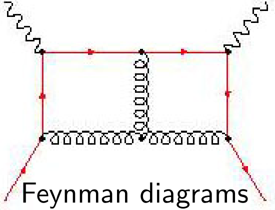

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$\downarrow$ DESY
Deutsches
Elektronen
Synchrotron

Simplification of Feynman sums

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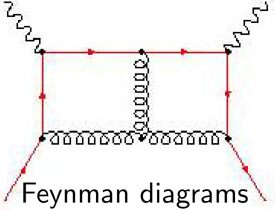

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Simplification of Feynman sums

XSummer using Form
(special purpose solver)

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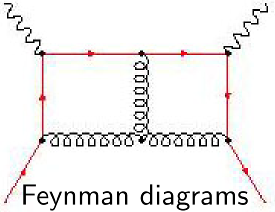

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GOAL: Evaluation of Feynman integrals

↓ DESY Deutsches Elektronen Synchrotron

Simplification of Feynman sums

→ XSummer using Form (special purpose solver)

→ Sigma

GIVEN

$$F(N)=\frac{\Gamma(2N)\Gamma(2-3\epsilon)\Gamma(N-2\epsilon+1)\Gamma(2(1-\epsilon))\Gamma(N-\epsilon+1)}{\Gamma(N)\Gamma(N-3\epsilon+2)\Gamma(1-2\epsilon)\Gamma(1-\epsilon)\Gamma(2(N-\epsilon+1))}\times$$
$$\times\left(2G+\sum_{i=1}^{N}\frac{\Gamma(i)\Gamma(i-3\epsilon+1)\Gamma(1-2\epsilon)\Gamma(1-\epsilon)\Gamma(2(i-\epsilon))}{\Gamma(2i)\Gamma(2-3\epsilon)\Gamma(i-2\epsilon+1)\Gamma(2(1-\epsilon))\Gamma(i-\epsilon)}X(i)\right)$$

with

$$G=g_0+g_1\epsilon+g_2\epsilon^2+g_3\epsilon^3+g_4\epsilon^4+O(\epsilon^5)$$

and

$$X(i)=x_0(i)+x_1(i)\epsilon+x_2(i)\epsilon^2+x_3(i)\epsilon^3+x_4(i)\epsilon^4+O(\epsilon^5)$$

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FIND the ϵ-expansion

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Sigma

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$$\times\left(2\boxed{G}+\boxed{\sum_{i=1}^{N}\frac{\Gamma(i)\Gamma(i-3\epsilon+1)\Gamma(1-2\epsilon)\Gamma(1-\epsilon)\Gamma(2(i-\epsilon))}{\Gamma(2i)\Gamma(2-3\epsilon)\Gamma(i-2\epsilon+1)\Gamma(2(1-\epsilon))\Gamma(i-\epsilon)}X(i)}\right)$$

1. FIND expansions for each box, e.g.,

$$\boxed{A(N)}=a_0(N)+a_1(N)\epsilon+a_2(N)\epsilon^2+a_3(N)\epsilon^3+a_4(N)\epsilon^4+O(\epsilon^5)$$

$$\boxed{B(N)}=b_0(N)+b_1(N)\epsilon+b_2(N)\epsilon^2+b_3(N)\epsilon^3+b_4(N)\epsilon^4+O(\epsilon^5)$$

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2. COMBINE:

$$A(N)+B(N)=\dots+(a_r(N)+b_r(N))\epsilon^r+\dots$$ component wise

$$A(N)\cdot B(N)=\dots+\Big(\sum_{l=0}^{r}a_l(N)b_{r-l}(N)\Big)\epsilon^r+\dots$$ Cauchy-product

$$F(N)=\boxed{\frac{\Gamma(2N)\Gamma(2-3\epsilon)\Gamma(N-2\epsilon+1)\Gamma(2(1-\epsilon))\Gamma(N-\epsilon+1)}{\Gamma(N)\Gamma(N-3\epsilon+2)\Gamma(1-2\epsilon)\Gamma(1-\epsilon)\Gamma(2(N-\epsilon+1))}}\times$$

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$$=$$

Sigma

$$F(N) = \boxed{\frac{\Gamma(2N)\Gamma(2-3\epsilon)\Gamma(N-2\epsilon+1)\Gamma(2(1-\epsilon))\Gamma(N-\epsilon+1)}{\Gamma(N)\Gamma(N-3\epsilon+2)\Gamma(1-2\epsilon)\Gamma(1-\epsilon)\Gamma(2(N-\epsilon+1))}} \times$$

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$$= \quad h_0(i) + h_1(i)\epsilon + h_2(i)\epsilon^2 + \dots$$

$$F(N) = \boxed{\frac{\Gamma(2N)\Gamma(2-3\epsilon)\Gamma(N-2\epsilon+1)\Gamma(2(1-\epsilon))\Gamma(N-\epsilon+1)}{\Gamma(N)\Gamma(N-3\epsilon+2)\Gamma(1-2\epsilon)\Gamma(1-\epsilon)\Gamma(2(N-\epsilon+1))}} \times$$

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$$= \underbrace{\sum_{i=1}^{N} h_0(i)}_{\text{sum 0}} + \epsilon \underbrace{\sum_{i=1}^{N} h_1(i)}_{\text{sum 1}} + \epsilon^2 \underbrace{\sum_{i=1}^{N} h_2(i)}_{\text{sum 2}} + \dots$$

Sigma

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$$= \boxed{f_0(N) + f_1(N)\epsilon + f_2(N)\epsilon^2 + f_3(N)\epsilon^3 + f_4(N)\epsilon^4 + O(N^5)}$$

COMBINE

Example 2: Padé approximation

Example 3

Quadratic Padé approximation to $\log(x)$ at $x = 1$

FIND $r_m(x) = \sum_{k=0}^{m} a_k x^k, \quad s_m(x) = \sum_{k=0}^{m} b_k x^k, \quad t_m(x) = \sum_{k=0}^{m} c_k x^k$:

$$r_m(x)\,(\log x)^2 + s_m(x)\,\log(x) + t_m(x) = O((x-1)^{3m+2}).$$

Quadratic Padé approximation to $\log(x)$ at $x = 1$

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A. Weideman finds

$$\begin{aligned} r_m(x) &= c_3 A(m,x) \\ s_m(x) &= c_2 A(m,x) + 2c_3 B(m,x) \\ t_m(x) &= c_1 A(m,x) + c_2 B(m,x) + c_3 C(m,x) \end{aligned}$$

where

$$A(m,x) = \sum_{k=0}^{m} \binom{m}{k}^3 (-x)^k \qquad B(m,x) = \sum_{k=0}^{m} \left[\frac{d}{dk}\binom{m}{k}^3\right](-x)^k$$

$$C(m,x) = \sum_{k=0}^{m} \left[\frac{d^2}{dk^2}\binom{m}{k}^3\right](-x)^k.$$

Quadratic Padé approximation to $\log(x)$ at $x = 1$

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$$C(m,x) = \sum_{k=0}^{m} \left[\frac{d^2}{dk^2}\binom{m}{k}^3\right](-x)^k.$$

Tests at $x = 1$, $m = 0, 1, \ldots$:
$c_1 = \pi^2, \quad c_2 = 0, \quad c_3 = 1$

For all $m \geq 0$,

$$\sum_{k=0}^{m}(-1)^k\Big[\pi^2\binom{m}{k}^3+\frac{d^2}{dk^2}\binom{m}{k}^3\Big]=0$$

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

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

Theorem (Sigma; 2002)

For all $m \geq 0$*,*

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

where

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

Proof.

Sigma

□

Zeilberger's creative telescoping paradigm

GIVEN

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

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

Zeilberger's creative telescoping paradigm

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

Sigma:

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

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

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

Zeilberger's creative telescoping paradigm

GIVEN

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

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:

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

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

Proving $\xrightarrow{\text{Sigma}}$ Finding

$$\sum_{k=0}^{2m}\binom{2m}{k}^3(-1)^kH_kH_{2m-k}=\frac{(3m)!(-1)^m}{m!m!m!}\frac{1}{12}\big(3H_m^2-6H_mH_{3m}+3H_{3m}^2+H_m^{(2)}$$
$$+12H_{2m}(H_{2m}+H_m-H_{3m})+4H_{2m}^{(2)}-3H_{3m}^{(2)}\big)$$

$$\sum_{k=0}^{2m}\binom{2m}{k}^3(-1)^kH_k^2=\frac{(3m)!(-1)^m}{m!m!m!}\frac{1}{12}\big(3H_m^2-6H_mH_{3m}+3H_{3m}^2-H_m^{(2)}$$
$$+12H_{2m}(H_{2m}+H_m-H_{3m})+2H_{2m}^{(2)}-3H_{3m}^{(2)}\big)$$

$$\sum_{k=0}^{2m}\binom{2m}{k}^3(-1)^kH_k^{(2)}=\frac{1}{2}\frac{(3m)!(-1)^m}{m!m!m!}(H_n^{(2)}+H_{2n}^{(2)})$$

Proving $\xrightarrow{\text{Sigma}}$ Finding

$$\sum_{k=0}^{2m}\binom{2m}{k}^3(-1)^k H_k H_{2m-k} = \frac{(3m)!(-1)^m}{m!m!m!}\frac{1}{12}\big(3H_m^2 - 6H_mH_{3m} + 3H_{3m}^2 + H_m^{(2)} + 12H_{2m}(H_{2m}+H_m-H_{3m}) + 4H_{2m}^{(2)} - 3H_{3m}^{(2)}\big)$$

$$\sum_{k=0}^{2m}\binom{2m}{k}^3(-1)^k H_k^2 = \frac{(3m)!(-1)^m}{m!m!m!}\frac{1}{12}\big(3H_m^2 - 6H_mH_{3m} + 3H_{3m}^2 - H_m^{(2)} + 12H_{2m}(H_{2m}+H_m-H_{3m}) + 2H_{2m}^{(2)} - 3H_{3m}^{(2)}\big)$$

$$\sum_{k=0}^{2m}\binom{2m}{k}^3(-1)^k H_k^{(2)} = \frac{1}{2}\frac{(3m)!(-1)^m}{m!m!m!}\big(H_n^{(2)} + H_{2n}^{(2)}\big)$$

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

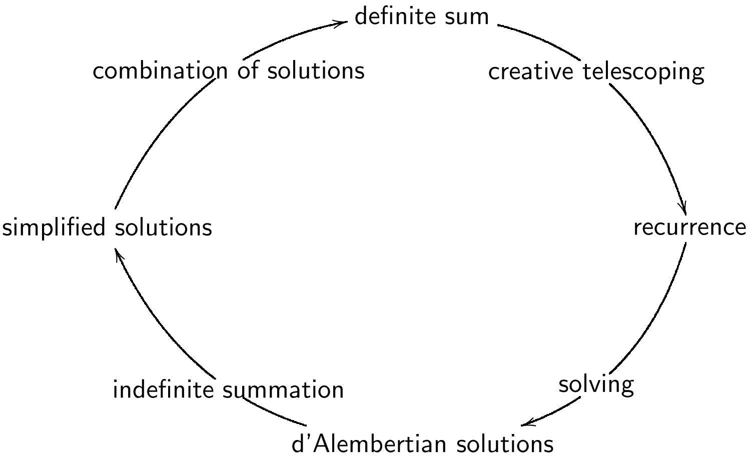
Proving $\xrightarrow{\text{Sigma}}$ Finding

$$\boxed{\sum_{k=0}^{2m}\binom{2m}{k}^3(-1)^k H_k H_{2m-k}} = \text{FIND}$$

$$\sum_{k=0}^{2m}\binom{2m}{k}^3(-1)^k H_k^2 = \frac{(3m)!(-1)^m}{m!m!m!}\frac{1}{12}\big(3H_m^2-6H_mH_{3m}+3H_{3m}^2-H_m^{(2)}$$
$$+12H_{2m}(H_{2m}+H_m-H_{3m})+2H_{2m}^{(2)}-3H_{3m}^{(2)}\big)$$

$$\sum_{k=0}^{2m}\binom{2m}{k}^3(-1)^k H_k^{(2)} = \frac{1}{2}\frac{(3m)!(-1)^m}{m!m!m!}(H_n^{(2)}+H_{2n}^{(2)})$$

The Sigma-summation spiral:



Weideman. Padé Approximations to the Logarithm I: Derivation via Differential Equations. 2005.

Driver, Prodinger, CS, Weideman. Padé approximations to the logarithm II: Identities, recurrences, and symbolic computation. 2006.

Driver, Prodinger, CS, Weideman. Padé approximations to the logarithm III: Alternative methods and additional results.

Krattenthaler. Private communication (differentiation, hypergeometric transformations).

Wenchang Chu. Harmonic number identities and Hermite-Padé approximation to the logarithm function. 2005.

Example 3:
Apéry's proof of the irrationality of $\zeta(3)$

Example 4

Apéry's proof (1979) of the irrationality of $\zeta(3)$ relies on the following fact:

$$a(n) = \sum_{k=0}^{n} \binom{n+k}{k}^2 \binom{n}{k}^2$$

and

$$b(n) = \sum_{k=0}^{n} \binom{n+k}{k}^2 \binom{n}{k}^2 \left(H_n^{(3)} + \sum_{m=1}^{k} \frac{(-1)^{m-1}}{2m^3 \binom{n+m}{m} \binom{n}{m}} \right)$$

satisfy both the recurrence relation

$$(n+1)^3 A(n) - (2n+3)\left(17n^2+51n+39\right) A(n+1) + (n+2)^3 A(n+2) = 0.$$

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Van der Poorten (1979) points out that Henri Cohen and Don Zagier showed this fact by

> *"some rather complicated but ingenious explanations"*

based on the creative telescoping method.

Apéry's proof (1979) of the irrationality of $\zeta(3)$ relies on the following fact:

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satisfy both the recurrence relation

$$(n+1)^3 A(n) - (2n+3)\left(17n^2 + 51n + 39\right) A(n+1) + (n+2)^3 A(n+2) = 0.$$

$a(n)$-case: trivial exercise by Zeilberger's algorithm (1991)

Apéry's proof (1979) of the irrationality of $\zeta(3)$ relies on the following fact:

$$a(n) = \sum_{k=0}^{n} \binom{n+k}{k}^2 \binom{n}{k}^2$$

and

$$b(n) = \sum_{k=0}^{n} \binom{n+k}{k}^2 \binom{n}{k}^2 \left(H_n^{(3)} + \sum_{m=1}^{k} \frac{(-1)^{m-1}}{2m^3 \binom{n+m}{m} \binom{n}{m}} \right)$$

satisfy both the recurrence relation

$$(n+1)^3 A(n) - (2n+3)\left(17n^2+51n+39\right) A(n+1) + (n+2)^3 A(n+2) = 0.$$

$b(n)$-case: skilful application of computer algebra

1. Generalization of the Cohen/Zagier method in the WZ-setting (Zeilberger, 1993)
2. Multi-summation + holonomic closure properties (Chyzak, 1998)

Apéry's proof (1979) of the irrationality of $\zeta(3)$ relies on the following fact:

$$a(n) = \sum_{k=0}^{n} \binom{n+k}{k}^2 \binom{n}{k}^2$$

and

$$b(n) = \sum_{k=0}^{n} \binom{n+k}{k}^2 \binom{n}{k}^2 \left(H_n^{(3)} + \sum_{m=1}^{k} \frac{(-1)^{m-1}}{2m^3 \binom{n+m}{m} \binom{n}{m}} \right)$$

satisfy both the recurrence relation

$$(n+1)^3 A(n) - (2n+3)\left(17n^2 + 51n + 39\right) A(n+1) + (n+2)^3 A(n+2) = 0.$$

$b(n)$*-case:* plain sailing (and not plane sailing) by Sigma

Example 4: Evaluation of a quadruple sum

Example 5

A challenging email (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:
```

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

```
Of course you can expand out the H's and get a quadruple sum.
There are zillions of ways to play with it, summing by parts, but
I have never managed to get rid of all the summations.

Robin
```

Simplify:

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

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

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

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

ζ-relations

This gives

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

E.g., in J.M. Borwein, Girgensohn. Evaluation of triple Euler sums, 1996.
Flajolet, Salvy. Euler sums and contour integral representations, 1998.
Granville. A decomposition of Riemann's zeta-function. 1997.
Zagier. Values of zeta functions and their applications. 1994.

we find

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

ζ-relations

Theorem.

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

Pemantle, CS. When is 0.999... equal to 1? 2007.

Panholzer, Prodinger. Computer-free evaluation of an infinite double sum. 2005.

Example 5: Particle physics II

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

GIVEN

$$F(N)=\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\underbrace{\left(\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(\varepsilon)\Gamma(1-\varepsilon)\frac{\Gamma(j+1-2\varepsilon)\Gamma(j+1+\varepsilon)\Gamma(k+j+1+N)}{\Gamma(j+1-\varepsilon)\Gamma(j+2+N)\Gamma(k+j+2)}\right.+\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(-\varepsilon)\Gamma(1+\varepsilon)\frac{\Gamma(j+1+2\varepsilon)\Gamma(j+1-\varepsilon)\Gamma(k+j+1+\varepsilon+N)}{\Gamma(j+1)\Gamma(j+2+\varepsilon+N)\Gamma(k+j+2+\varepsilon)}\left.\right)}_{f(N,k,j)}.$$

GIVEN

$$F(N) = \sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Bigg(\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(\varepsilon)\Gamma(1-\varepsilon)\frac{\Gamma(j+1-2\varepsilon)\Gamma(j+1+\varepsilon)\Gamma(k+j+1+N}{\Gamma(j+1-\varepsilon)\Gamma(j+2+N)\Gamma(k+j+2)}$$

$$\underbrace{+\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(-\varepsilon)\Gamma(1+\varepsilon)\frac{\Gamma(j+1+2\varepsilon)\Gamma(j+1-\varepsilon)\Gamma(k+j+1+\varepsilon+N)}{\Gamma(j+1)\Gamma(j+2+\varepsilon+N)\Gamma(k+j+2+\varepsilon)}}_{f(N,k,j)}\Bigg).$$

FIND the ϵ-expansion

$$F(N) = F_0(N) + \varepsilon F_1(N) + \dots$$

GIVEN

$$F(N)=\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\underbrace{\Bigg(\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(\varepsilon)\Gamma(1-\varepsilon)\frac{\Gamma(j+1-2\varepsilon)\Gamma(j+1+\varepsilon)\Gamma(k+j+1+N}{\Gamma(j+1-\varepsilon)\Gamma(j+2+N)\Gamma(k+j+2)} + \frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(-\varepsilon)\Gamma(1+\varepsilon)\frac{\Gamma(j+1+2\varepsilon)\Gamma(j+1-\varepsilon)\Gamma(k+j+1+\varepsilon+N)}{\Gamma(j+1)\Gamma(j+2+\varepsilon+N)\Gamma(k+j+2+\varepsilon)}\Bigg)}_{f(N,k,j)}$$

Step 1: FIND the ϵ-expansion

$$f(N,k,j)= \qquad f_0(N,k,j)+ \qquad \varepsilon f_1(N,k,j)+\dots$$

GIVEN

$$F(N)=\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Bigg(\underbrace{\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(\varepsilon)\Gamma(1-\varepsilon)\frac{\Gamma(j+1-2\varepsilon)\Gamma(j+1+\varepsilon)\Gamma(k+j+1+N}{\Gamma(j+1-\varepsilon)\Gamma(j+2+N)\Gamma(k+j+2)} +\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(-\varepsilon)\Gamma(1+\varepsilon)\frac{\Gamma(j+1+2\varepsilon)\Gamma(j+1-\varepsilon)\Gamma(k+j+1+\varepsilon+N)}{\Gamma(j+1)\Gamma(j+2+\varepsilon+N)\Gamma(k+j+2+\varepsilon)}}_{f(N,k,j)}\Bigg)$$

Step 2: Simplify the sums in

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}f(N,k,j)=\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}f_0(N,k,j)+\varepsilon\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}f_1(N,k,j)+\dots$$

$$||$$

$$F(N)$$

GIVEN

$$F(N) = \sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Bigg(\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(\varepsilon)\Gamma(1-\varepsilon)\frac{\Gamma(j+1-2\varepsilon)\Gamma(j+1+\varepsilon)\Gamma(k+j+1+N}{\Gamma(j+1-\varepsilon)\Gamma(j+2+N)\Gamma(k+j+2)}$$

$$\underbrace{+\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(-\varepsilon)\Gamma(1+\varepsilon)\frac{\Gamma(j+1+2\varepsilon)\Gamma(j+1-\varepsilon)\Gamma(k+j+1+\varepsilon+N)}{\Gamma(j+1)\Gamma(j+2+\varepsilon+N)\Gamma(k+j+2+\varepsilon)}}_{f(N,k,j)}\Bigg)$$

Step 2: Simplify the sums in

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f(N,k,j) = \sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j) + \varepsilon \sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_1(N,k,j) + \dots$$

$$||$$

$$F(N)$$

Simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j)$$

$$\sum_{j=0}^{a} f_0(N,k,j) =$$ ▸ Sigma

Simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j)$$

$$\sum_{j=0}^{a} f_0(N,k,j) = \frac{(a+1)!(k-1)!(a+k+N+1)!(H_a - H_{a+k} - H_{a+N} + H_{a+k+N})}{N(a+k+1)!(a+N+1)!(k+N+1)!}$$

$$+ \frac{H_k + S_N - H_{k+N}}{kN(k+N+1)N!} + \frac{(2a+k+N+2)a!k!(a+k+N)!}{(a+k+1)(a+N+1)(a+k+1)!(a+N+1)!(k+N+1)!}$$

Simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j)$$

$$\sum_{j=0}^{\infty} f_0(N,k,j) = \qquad \frac{H_k + H_N - H_{k+N}}{kN(k+N+1)N!}$$

Simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j)$$

$$\sum_{k=1}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j) = \sum_{k=1}^{\infty}\frac{H_k + H_N - H_{k+N}}{kN(k+N+1)N!}$$

Simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j)$$

$$\sum_{k=1}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j) = \sum_{k=1}^{\infty}\frac{H_k + H_N - H_{k+N}}{kN(k+N+1)N!}$$

$$= \text{Sigma}$$

Simplify

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j)$$

$$\sum_{k=1}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j) = \sum_{k=1}^{\infty}\frac{H_k+H_N-H_{k+N}}{kN(k+N+1)N!}$$

$$= \frac{H_N^2+H_N^{(2)}}{2N(N+1)!}$$

where

$$H_N^{(2)} = \sum_{i=1}^{N}\frac{1}{i^2}$$

GIVEN

$$F(N) = \sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Bigg(\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(\varepsilon)\Gamma(1-\varepsilon)\frac{\Gamma(j+1-2\varepsilon)\Gamma(j+1+\varepsilon)\Gamma(k+j+1+N}{\Gamma(j+1-\varepsilon)\Gamma(j+2+N)\Gamma(k+j+2)}$$

$$+\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(-\varepsilon)\Gamma(1+\varepsilon)\frac{\Gamma(j+1+2\varepsilon)\Gamma(j+1-\varepsilon)\Gamma(k+j+1+\varepsilon+N)}{\Gamma(j+1)\Gamma(j+2+\varepsilon+N)\Gamma(k+j+2+\varepsilon)}\Bigg)$$

$$=\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j)+\varepsilon\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_1(N,k,j)+\dots,$$

Sigma computes

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty} f_0(N,k,j)=\frac{H_N^2+3H_N}{2N(N+1)!}.$$

GIVEN

$$F(N)=\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}\Bigg(\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(\varepsilon)\Gamma(1-\varepsilon)\frac{\Gamma(j+1-2\varepsilon)\Gamma(j+1+\varepsilon)\Gamma(k+j+1+N}{\Gamma(j+1-\varepsilon)\Gamma(j+2+N)\Gamma(k+j+2)}$$

$$+\frac{\Gamma(k+1)}{\Gamma(k+2+N)}\Gamma(-\varepsilon)\Gamma(1+\varepsilon)\frac{\Gamma(j+1+2\varepsilon)\Gamma(j+1-\varepsilon)\Gamma(k+j+1+\varepsilon+N)}{\Gamma(j+1)\Gamma(j+2+\varepsilon+N)\Gamma(k+j+2+\varepsilon)}\Bigg)$$

$$=\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}f_0(N,k,j)+\varepsilon\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}f_1(N,k,j)+\dots,$$

Sigma computes

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}f_0(N,k,j)=\frac{H_N^2+3H_N}{2N(N+1)!}.$$

$$\sum_{k=0}^{\infty}\sum_{j=0}^{\infty}f_1(N,k,j)=\frac{-H_N^3-3H_NH_N^{(2)}-8H_N}{6N(N+1)!}.$$

Appendix

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

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

◂ Back

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

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

Denominator bound: COMPUTE a polynomial $d \in \mathbb{Q}(k)[h]$:

$$\boxed{d = 1}$$

$$\forall g \in \mathbb{Q}(k)(h): \quad \sigma(g) - g = h \quad \Rightarrow \quad g\,d \in \mathbb{Q}(k)[h].$$

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

$$\sigma(\frac{g'}{d}) - \frac{g'}{d} = h.$$

Back

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

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

Denominator bound: COMPUTE a polynomial $d \in \mathbb{Q}(k)[h]$:

$d = 1$

$$\forall g \in \mathbb{Q}(k)(h): \quad \sigma(g) - g = h \quad \Rightarrow \quad g\,d \in \mathbb{Q}(k)[h].$$

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

$$\sigma(\frac{g'}{d}) - \frac{g'}{d} = h.$$

Degree bound: COMPUTE $b \geq 0$:

$b = 2$

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

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

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Denominator bound: COMPUTE a polynomial $d \in \mathbb{Q}(k)[h]$:

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Polynomial Solution: FIND

g=hk-k

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

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

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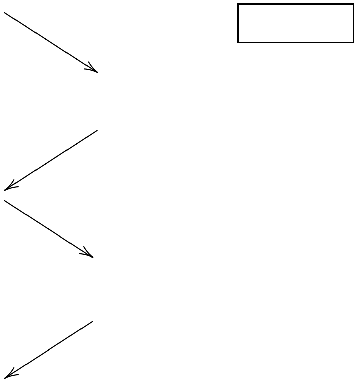

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$c=0$, $g_1 = k+d$, $d\in\mathbb{Q}$

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

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coeff. comp. →

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

$$g_0 = -k,\ d = 0 \quad\longleftarrow\quad \boxed{\sigma(g_0)-g_0 = -1 - d\frac{1}{k+1}}$$

Back

The general case (Karr's algorithm; 1981)

GIVEN a $\Pi\Sigma$-field $(\mathbb{F}, \sigma)$:
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\sigma(t_3) &= \alpha_3\, t_3 + \beta_3, & \alpha_3 &\in \mathbb{K}(t_1,t_2)^*, & \beta_3 &\in \mathbb{K}(t_1,t_2) \\
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GIVEN $f \in \mathbb{F}$;

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

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