RISC/SCIEnce Training School in Symbolic Computation

Sigma - A package for multi-summation

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Some literature:

M. Karr. Summation in finite terms. *J. ACM*, 28:305–350, 1981.

C. Schneider. Symbolic summation assists combinatorics. *Sém. Lothar. Combin.*, 56:1–35, 2007.
Available at `http://www.mat.univie.ac.at/~slc/`

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

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

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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

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

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

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Try it out!

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

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

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

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

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

Telescoping in the given difference field

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

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

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with

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

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with

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Hence,

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

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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

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

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

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

Degree bound: COMPUTE $b \geq 0$:

$$\boxed{b = 2}$$

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

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

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

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

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$d=1$

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

Degree bound: COMPUTE $b\geq 0$:

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

$b=2$

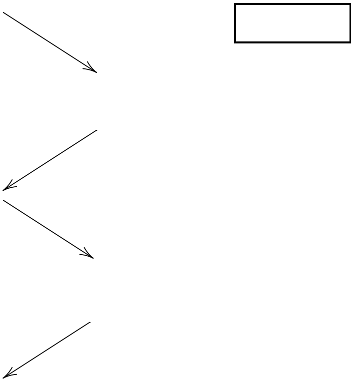
Polynomial Solution: FIND

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

g=hk-k

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

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



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

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

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coeff. comp.

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

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

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

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

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

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

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

coeff. comp.

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

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

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

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

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g=hk-k

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

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

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

The general case (Karr's algorithm)

GIVEN a $\Pi\Sigma$-field $(\mathbb{F},\sigma)$:
a rational function field $\mathbb{F} := \mathbb{K}(t_1)(t_2)\dots(t_e)$ with an automorphism

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GIVEN a $\Pi\Sigma$-field $(\mathbb{F},\sigma)$:
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$$\sigma(c)=c\quad\forall c\in\mathbb{K}$$

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such that $\{c \in \mathbb{K}(t_1)\dots(t_e) | \sigma(c) = c\} = \mathbb{K}$.

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GIVEN $f \in \mathbb{F}$;

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

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

telescoping

- GIVEN
$$\sum_{k=0}^{n} f(k).$$
- FIND $g(k)$:
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- THEN (with some mild extra conditions)

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

Refined telescoping

- GIVEN

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

- FIND $g(k)$ 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)

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

Degree optimal w.r.t the top extension

$$\sum_{k=1}^{n}\frac{1}{k(k+1)^2(k+2)^3} =$$

$$\sum_{k=2}^{n}\frac{2-kH_k+H_k^4-kH_k^5}{H_k-kH_k^2} =$$

Sigma

$$\sum_{k=1}^{n}H_k^4 =$$

Degree optimal w.r.t the top extension

$$\sum_{k=1}^{n}\frac{1}{k(k+1)^2(k+2)^3}=-\frac{1}{4}\sum_{k=1}^{n}\frac{9k+2}{k^3}+\frac{n\left(69n^5+585n^4+1967n^3+3283n^2+2728n+904\right)}{16(n+1)^3(n+2)^3}$$

$$\sum_{k=2}^{n}\frac{2-kH_k+H_k^4-kH_k^5}{H_k-kH_k^2}=\sum_{k=2}^{n}\frac{k^2+H_k}{k^2H_k}+(n+1)H_n^3-(2n+1)\left(\tfrac{3}{2}H_n^2-3H_n+\tfrac{3}{2}\right)+\frac{1}{H_n}$$

$$\sum_{k=1}^{n}H_k^4=-H_n^{(3)}-2H_n^{(2)}+2\sum_{k=1}^{n}\frac{H_k}{k^2}+(n+1)H_n^4-2(2n+1)H_n^3+6(2n+1)H_n^2-12(2n+1)H_n+24n.$$

Further examples

$$\sum_{k=1}^{n}\frac{k+1}{k(k+2)}=-\frac{n(3n+5)}{4(n+1)(n+2)}+\sum_{k=1}^{n}\frac{1}{k}$$

$$\sum_{k=2}^{n}\frac{1}{k(k-1)2^k}=\frac{-1}{n2^{n+1}}+\frac{1}{4}-\frac{1}{2}\sum_{k=2}^{n}\frac{1}{k2^k}$$

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

$$\sum_{k=2}^{n}\frac{(k+1)\left(k(k+1)^2(k+2)H_k^3+k\left(3k^2+8k+5\right)H_k^2-(k+2)H_k-k-2\right)}{H_k\left(k(k+1)^2(k+2)H_k^3+2\left(k^3+2k^2-1\right)H_k^2-\left(k^2+5k+5\right)H_k-2k-3\right)}$$
$$=\frac{-6(n+1)(n+2)H_n^2-6(2n+3)H_n+11(n+1)(n+2)}{11H_n\left(2n+(n+1)(n+2)H_n+3\right)}+\sum_{k=2}^{n}\frac{k(k+1)}{kH_k-1}$$

The analogue problem for Π-extensions

$$\prod_{k=1}^{n}\frac{(-k-1)(k+7)}{(k+4)^2}=\frac{4}{35}\,\frac{(n+5)(n+6)(n+7)}{(n+2)(n+3)(n+4)}\,(-1)^n,$$

$$\prod_{k=1}^{n}\frac{(k+3)(H_k(k+1)+1)^2(H_k(k+2)(k+1)+2k+3)}{(k+1)^2H_k(H_k(k+3)(k+2)(k+1)+3(k+4)k+11)}$$
$$=\frac{11}{6}\,\frac{(n+3)(n+2)(H_n(n+1)+1)^2}{(n+1)(H_n(n+3)(n+2)(n+1)+3(n+4)n+11)}\prod_{k=1}^{n}H_k,$$

$$\prod_{k=1}^{n}\frac{k!(H_k(k+2)(k+1)+2k+3)(H_k(k+1)+1)}{H_k(k+3)(k+2)(k+1)+3(k+4)k+11}$$
$$=\frac{11(H_n(n+1)+1)}{H_n(n+3)(n+2)(n+1)+3(n+4)n+11}\prod_{k=1}^{n}k!H_k,$$

$$\prod_{k=1}^{n}\frac{(q^{k+2}+(k+1)!)(q^{k+1}+k!)(k+2)(k+1)}{(q^{k+3}+(k+2)!)(k+3)}$$
$$=\frac{3(q^3+2)}{q+1}\,\frac{(q^{n+1}(n+1)+(n+1)!)}{(q^{n+3}+(n+2)!)(n+3)}\prod_{k=1}^{n}(kq^k+k!)$$

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

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

Simpler w.r.t. the depth

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

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

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

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

Simpler w.r.t. the depth

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

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

$$\sum_{k=1}^{n} \frac{\sum_{j=1}^{k} \frac{H_j}{j^2}}{k^3} = S(3,2,1,N) \qquad \text{(Harmonic sum)}$$

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

Further examples

$$\sum_{k=1}^{n} H_k^3 = \frac{1}{2}\Big(2(n+1)H_n^3 - 3(2n+1)H_n^2 + 6(2n+1)H_n - 12n - 1 + H_n^{(2)}\Big)$$

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

$$\sum_{k=1}^{n}\left(\sum_{j=1}^{k}\frac{H_j^{(2)}}{j^3}\right)^2 = -\left({H_n^{(2)}}^2 + H_n^{(4)}\right)\sum_{j=1}^{n}\frac{H_j^{(2)}}{j^3} + (n+1)\left(\sum_{j=1}^{n}\frac{H_j^{(2)}}{j^3}\right)^2 + \sum_{j=1}^{n}\frac{{H_j^{(2)}}^3}{j^3} - \sum_{j=1}^{n}\frac{{H_j^{(2)}}^2}{j^5} + \sum_{j=1}^{n}\frac{H_j^{(2)}H_j^{(4)}}{j^3}.$$

Creative telescoping (for order 2)

GIVEN

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

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

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

$$=\boxed{c_0(n)f(n,k)+c_1(n)f(n+1,k)+c_2(n)f(n+2,k).}$$

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$$= \boxed{c_0(n) f(n,k) + c_1(n) f(n+1,k) + c_2(n) f(n+2,k).}$$

THEN summation over k from 0 to n gives

$$\boxed{g(n,n+1) - g(n,0)}$$
$$= \boxed{\begin{array}{l} c_0(n)\,\mathsf{S}(n) + \\ c_1(n)\left[\mathsf{S}(n+1) - f(n+1,n+1)\right] \\ c_2(n)\left[\mathsf{S}(n+2) - f(n+2,n+1) - f(n+2,n+2)\right]. \end{array}}$$

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HENCE

$$h(n) = c_0(n)S(n) + c_1(n)S(n+1) + c_2(n)S(n+2)$$

for some $h(n)$.

Creative telescoping (for order 2)

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HENCE

$$h(n)=c_0(n)S(n)+c_1(n)S(n+1)+c_2(n)S(n+2)$$

for some $h(n)$.

Example with $S(n)=\sum_{k=0}^{n}\binom{n}{k}H_k$

FIND a recurrence for

$$S(n) := \sum_{k=1}^{n} \binom{n}{k} H_k.$$

A difference field for the summand

Consider the rational function field

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

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

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

REPRESENT $f(n+i,k)$ in $\mathbb{F}$:

$$f(n,k) = \mathsf{H}_k \binom{n}{k} \quad \longleftrightarrow \quad h\,b =: f_0$$

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$$f(n+2,k) = \frac{(n+1)\,(n+2)\,\mathsf{H}_k \binom{n}{k}}{(n+1-k)\,(n+2-k)} \quad \longleftrightarrow \quad \frac{(n+1)\,(n+2)\,h\,b}{(n+1-k)\,(n+2-k)} =: f_2.$$

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FIND $c_0,c_1,c_2\in\mathbb{Q}(n)$ and $g\in\mathbb{F}$:

$$\boxed{\sigma(g)-g=c_0f_0+c_1f_1+c_2f_2.}$$

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FIND $c_0,c_1,c_2\in\mathbb{Q}(n)$ and $g\in\mathbb{F}$:

$$\boxed{\sigma(g)-g=c_0f_0+c_1f_1+c_2f_2.}$$

Sigma computes

$$c_0:=4\,(1+n),\quad c_1:=-2\,(3+2\,n),\quad c_2:=2+n,$$

$$g:=\frac{(1+n)\,(-2+k-n+(2\,k-2\,k^2+k\,n)h)\,b)}{(1-k+n)\,(2-k+n)}.$$

REPRESENT $f(n+i,k)$ in $\mathbb{F}$:

$$f(n,k) = \mathsf{H}_k \binom{n}{k} \quad \longleftrightarrow \quad h\,b =: f_0$$

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$$f(n+2,k) = \frac{(n+1)\,(n+2)\,\mathsf{H}_k \binom{n}{k}}{(n+1-k)\,(n+2-k)} \quad \longleftrightarrow \quad \frac{(n+1)\,(n+2)\,h\,b}{(n+1-k)\,(n+2-k)} =: f_2.$$

This gives

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

with

$$c_0(n) := 4\,(1+n), \quad c_1(n) := -2\,(3+2\,n), \quad c_2(n) := 2+n,$$

$$g(n,k) := \frac{(1+n)\,(-2+k-n+(2\,k-2\,k^2+k\,n)H_k)\,\binom{n}{k})}{(1-k+n)\,(2-k+n)}.$$

REPRESENT $f(n+i,k)$ in $\mathbb{F}$:

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$$f(n+2,k) = \frac{(n+1)\,(n+2)\,\mathsf{H}_k\binom{n}{k}}{(n+1-k)\,(n+2-k)} \quad \longleftrightarrow \quad \frac{(n+1)\,(n+2)\,h\,b}{(n+1-k)\,(n+2-k)} =: f_2.$$

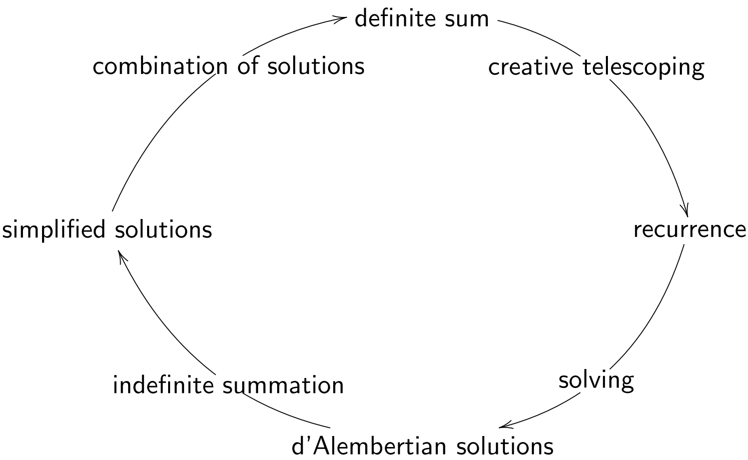
Summing over k from 0 to n gives

$$\boxed{1 = 4(1+n)S(n) - 2(3+2n)S(n+1) + (2+n)S(n+2)}$$

for

$$S(n) = \sum_{k=0}^{n}\binom{n}{k}H_k.$$

The Sigma-summation spiral:



Examples