

IMA Summer Program
Special Functions in the Digital Age
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Sigma: A Summation Package for Discovering and Proving

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PART I: Discovering Sum Identities

A Bonus Problem in "Concrete Mathematics"

Chapter 6. Special Numbers, Bonus Problem 69:

Find a closed form for

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

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

Knuth's answer to the problem is

$$-\frac{1}{36} n (-1 + 9n + 10n^2) + \frac{1}{3} n \left(\frac{1}{2} + n\right) (1 + n) (-H_n + 2H_{2n})$$



with the remark

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



<< Sigma`

Sigma - A summation package by Carsten
Schneider - © RISC Linz - V 1.01 β (12 / 06 / 02)

mySum = SigmaSum[k^2 SigmaHNumber[n + k], {k, 1, n}]

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

SigmaReduce[mySum]

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



All objects are nested sums and products

$$\sum_{k=1}^n k^2 H_{k+n} \text{ // GetFullDefinition}$$

$$\sum_{k=1}^n k^2 \left(H_n + \sum_{o_1=1}^k \frac{1}{n + o_1} \right)$$

GetDefinition[$\left(\frac{n}{k}\right)$, k]

$$\prod_{o_1=1}^k \left(\frac{1 + n - o_1}{o_1} \right)$$



Two worlds:

ring of sequences $\mathbb{K}^{\mathbb{N}}$ $\xleftarrow{\text{automatic translation}}$ $\Pi\Sigma$ -fields

The user is dispensed from difference field theory (C.S.)

Solving first order linear difference equations in $\Pi\Sigma$ -fields (Karr, 1981)



Simplified version (C.S.)

Calkin's Identity

PROBLEM: Find a closed form for

$$\sum_{k=0}^n \left(\sum_{j=0}^k \binom{n}{j} \right)^3$$

▼ Case 1:

$$\text{mySum} = \sum_{k=0}^a \left(\sum_{j=0}^k \binom{n}{j} \right) \mathbf{1};$$

`res = SigmaReduce[mySum]`

$$\frac{1}{2} \left((-a + n) \binom{n}{a} + (2 + 2a - n) \sum_{\ell_1=0}^a \binom{n}{\ell_1} \right)$$



res = res /. {a -> n}

$$\frac{1}{2} (2 + n) \sum_{l_1=0}^n \binom{n}{l_1}$$

res /. { $\sum_{l_1=0}^n \binom{n}{l_1} \rightarrow 2^n$ **}**

$$\frac{1}{2} (2 + n) 2^n$$

▼ Case 2:

$$\text{mySum} = \sum_{k=0}^a \left(\sum_{j=0}^k \binom{n}{j} \right)^2 ;$$

SigmaReduce[mySum]

$$\sum_{l_1=0}^a \left(\sum_{l_2=0}^{l_1} \binom{n}{l_2} \right)^2$$



Generalized summation algorithm (C.S.):

Simplify nested multisums **by** appropriate sum **extensions**

res = SigmaReduce[mySum, SimplifyByExt -> Depth]

$$\frac{1}{2} \left(-2 (a - n) \binom{n}{a} \sum_{l_1=0}^a \binom{n}{l_1} + \right. \\ \left. (2 + 2 a - n) \left(\sum_{l_1=0}^a \binom{n}{l_1} \right)^2 - n \sum_{l_1=0}^a \left(\binom{n}{l_1} \right)^2 \right)$$



res = res /. {a -> n}

$$\frac{1}{2} \left((2+n) \left(\sum_{l_1=0}^n \binom{n}{l_1} \right)^2 - n \sum_{l_1=0}^n \left(\binom{n}{l_1} \right)^2 \right)$$

res /. { $\sum_{l_1=0}^n \binom{n}{l_1} \rightarrow 2^n$ **,** $\sum_{l_1=0}^n \left(\binom{n}{l_1} \right)^2 \rightarrow \binom{2n}{n}$ **}**

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

▼ Case 3: (Calkin's Identity)

$$\text{mySum} = \sum_{k=0}^n \left(\sum_{j=0}^k \binom{n}{j} \right)^3 ;$$

• Finding a recurrence

rec = GenerateRecurrence[mySum, RecOrder -> 2]

Order: 2

Solution!

$$\left\{ 4(1+2n) \text{SUM}[n] + (12+7n) \text{SUM}[1+n] + (-1-n) \text{SUM}[2+n] == -2(-10+9n) \left(\sum_{l_1=0}^n \binom{n}{l_1} \right)^3 \right\}$$

- Z's creative telescoping trick can be applied in $\Pi\Sigma$ -fields(C.S.)

→ Recurrences for nested multisums can be computed



$$\text{rec} = \text{rec} / \cdot \left\{ \sum_{l_1=0}^n \binom{n}{l_1} \cdot \rightarrow 2^n \right\}$$

$$\{4(1+2n) \text{SUM}[n] + (12+7n) \text{SUM}[1+n] + (-1-n) \text{SUM}[2+n] == -2(-10+9n)(2^n)^3\}$$

• Solving the recurrence

recSol =

$$\text{SolveRecurrence}[\text{rec}[[1]], \text{SUM}[n], \text{Tower} \rightarrow \left\{ \binom{2n}{n} \right\}]$$

$$\left\{ \left\{ 0, n \binom{2n}{n} \cdot 2^n \right\}, \left\{ 1, \frac{1}{2} (2+n) (2^n)^3 \right\} \right\}$$



- Solving of linear difference equations in $\Pi\Sigma$ -fields(C.S.)

first order \longrightarrow arbitrary order

\rightarrow Recurrences can be solved in terms of nested multisums

• Finding the linear combination

FindLinearCombination[recSol, mySum, 2]

$$-\frac{3}{4} n \binom{2n}{n} \cdot 2^n + \frac{1}{2} (2+n) (2^n)^3$$

We obtain for all $n \geq 0$:

$$\sum_{k=0}^n \left(\sum_{j=0}^k \binom{n}{j} \right)^3 = -\frac{3}{4} n \binom{2n}{n} 2^n + \frac{1}{2} (2+n) (2^n)^3$$

Krattenthaler – Example

PROBLEM: Find a closed form for

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

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

(The number of rhombus tilings of a symmetric hexagon, Fulmek&Krattenthaler)

▼ Sum 1

$$\text{mySum1} = \sum_{k=1}^n - \frac{H_k (3+k+n)! (-1)^k (-1)^n}{(1+k)! (2+k)! (-k+n)!};$$

• Finding a recurrence

```
rec1 = GenerateRecurrence[mySum1, RecOrder -> 3]
```

```
Order: 3
```

```
Solution!
```

$$\{n (1+n) (2+n)^2 (3+n) (4+n)^2 (9+2n) (-1+n)! \cdot \text{SUM}[n] -$$

$$n (1+n) (2+n) (3+n) (4+n) (9+2n)$$

$$(13+8n+n^2) (-1+n)! \cdot \text{SUM}[1+n] -$$

$$n (1+n) (2+n) (3+n) (4+n) (5+2n) (6+6n+n^2)$$

$$(-1+n)! \cdot \text{SUM}[2+n] + n (1+n) (2+n) (3+n)^2$$

$$(4+n) (5+n) (5+2n) (-1+n)! \cdot \text{SUM}[3+n] ==$$

$$-2 (5+2n) (7+2n) (9+2n) (4+n)! \cdot (-1)^n\}$$

• Solving the recurrence

```
SolveRecurrence[rec1[[1]], SUM[n]]
```

```
{{0, 1}, {0, (2+n) (-1)^n}}
```



Solving the recurrence with sum extensions

```
recSol = SolveRecurrence[
  rec1[[1]], SUM[n], NestedSumExt -> Infinity,
  AlgebraicRelationInSumSolutions -> True]
```

$$\left\{ \{0, 1\}, \{0, (2+n)(-1)^n\}, \right. \\ \left. \left\{0, -\sum_{\ell_1=0}^n (3+2\ell_1)(-1)^{\ell_1} \sum_{\ell_2=1}^{\ell_1} \frac{(-1)^{\ell_2}}{\ell_2(2+\ell_2)}\right\}, \right. \\ \left. \left\{1, 2 \sum_{\ell_1=0}^n (3+2\ell_1)(-1)^{\ell_1} \sum_{\ell_2=1}^{\ell_1} \frac{1+\ell_2}{\ell_2(2+\ell_2)}\right\} \right\}$$

```
FindLinearCombination[recSol, mySum1, 3]
```

$$2 \sum_{\ell_1=0}^n (3+2\ell_1)(-1)^{\ell_1} \sum_{\ell_2=1}^{\ell_1} \frac{1+\ell_2}{\ell_2(2+\ell_2)} - \\ 2 \sum_{\ell_1=0}^n (3+2\ell_1)(-1)^{\ell_1} \sum_{\ell_2=1}^{\ell_1} \frac{(-1)^{\ell_2}}{\ell_2(2+\ell_2)}$$

↘

Elimination of algebraic relations

```
SolveRecurrence[rec1[[1]],
  SUM[n], NestedSumExt -> Infinity]
```

$$\left\{ \{0, 1\}, \{0, (2+n)(-1)^n\}, \right. \\ \left. \left\{0, \frac{n-2(1+n) \sum_{\ell_1=1}^n \frac{1+\ell_1}{\ell_1(2+\ell_1)}}{2(1+n)}\right\}, \left\{1, \right. \right. \\ \left. \left. \frac{(3+3n+n^2)(-1)^n + 2(1+n)(2+n)^2(-1)^n \sum_{\ell_1=1}^n \frac{1+\ell_1}{\ell_1(2+\ell_1)}}{(1+n)(2+n)} \right\} \right\}$$



$$\text{SigmaReduce} \left[\sum_{\iota_1=1}^n \frac{1 + \iota_1}{\iota_1 (2 + \iota_1)}, \right. \\ \left. \text{SimpleSumRepresentation} \rightarrow \text{True} \right]$$

$$\frac{-n (5 + 3 n) + 4 (1 + n) (2 + n) \sum_{\iota_1=1}^n \frac{1}{\iota_1}}{4 (1 + n) (2 + n)}$$



Solving the recurrence with Harmonic numbers

```
recSol1 =
  SolveRecurrence[rec1[[1]], SUM[n], Tower -> {Hn}]
```

$$\left\{ \{0, 1\}, \left\{ 0, \frac{-n (9 + 5 n) + 4 (1 + n) (2 + n) H_n}{(1 + n) (2 + n)} \right\}, \right. \\ \left. \{0, (2 + n) (-1)^n\}, \left\{ 1, \frac{(-n (32 + 33 n + 9 n^2) + 8 (1 + n) (2 + n)^2 H_n) (-1)^n}{4 (1 + n) (2 + n)} \right\} \right\}$$

• Finding the linear combination

```
solution1 = FindLinearCombination[recSol1, mySum1, 3] //
  SigmaSimplify
```

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

▼ Sum 2

$$\text{mySum2} = \sum_{k=1}^n - \frac{(3 + k + n) ! \cdot (-1)^k (1 - (2 + n) (-1)^n)}{k ((1 + k) !)^2 (-k + n) !} ;$$

• Finding a recurrence

```
rec2 = GenerateRecurrence[mySum2, RecOrder -> 2]
```

```
Order: 2
```

```
Solution!
```

$$\left\{ n (1+n) (3+n) (4+n) (7+2n) (-1+n) ! \cdot \right. \\ (1 + (3+n) (-1)^n) (-1 + (4+n) (-1)^n) \text{SUM}[n] - \\ 6n (1+n) (3+n)^2 (-1+n) ! \cdot (-1 + (2+n) (-1)^n) \\ (-1 + (4+n) (-1)^n) \text{SUM}[1+n] - n (1+n) (-1+n) ! \cdot \\ \left. (- (2+n) (3+n) (5+2n) - (2+n) (3+n) (5+2n) (-1)^n + \right. \\ (2+n)^2 (3+n)^2 (5+2n) ((-1)^n)^2) \text{SUM}[2+n] = = \\ 2 (4+n) ! \cdot ((5+2n) (7+2n) - (3+n) (5+2n) (7+2n) \\ (-1)^n - (5+2n) (7+2n) (10+6n+n^2) ((-1)^n)^2 + \\ \left. (2+n) (3+n) (4+n) (5+2n) (7+2n) ((-1)^n)^3 \right\}$$

```
rec2 = rec2[[1]] /. {((-1)^n)^3 -> (-1)^n, ((-1)^n)^2 -> 1}
```

$$n (1+n) (3+n) (4+n) (7+2n) (-1+n) ! \cdot \\ (1 + (3+n) (-1)^n) (-1 + (4+n) (-1)^n) \text{SUM}[n] - \\ 6n (1+n) (3+n)^2 (-1+n) ! \cdot (-1 + (2+n) (-1)^n) \\ (-1 + (4+n) (-1)^n) \text{SUM}[1+n] - n (1+n) (-1+n) ! \cdot \\ (- (2+n) (3+n) (5+2n) + (2+n)^2 (3+n)^2 (5+2n) - \\ (2+n) (3+n) (5+2n) (-1)^n) \text{SUM}[2+n] = = 2 (4+n) ! \cdot \\ ((5+2n) (7+2n) - (5+2n) (7+2n) (10+6n+n^2) - \\ (3+n) (5+2n) (7+2n) (-1)^n + \\ (2+n) (3+n) (4+n) (5+2n) (7+2n) (-1)^n)$$

• *Solving the recurrence*

```
SolveRecurrence[rec2, SUM[n],
  NestedSumExt -> Infinity, WithMinusPower -> True]
{ {0, -n (2 + n) (4 + n) + (9 + 28 n + 23 n2 + 8 n3 + n4) (-1)n },
  {0, -(2 + n) (-941 + 108 n + 27 n2) +
    (-698 + 756 n + 621 n2 + 216 n3 + 27 n4) (-1)n },
  {1,  $\frac{1}{3} \left( -(1 + 3 n + n^2) (9 + 28 n + 23 n^2 + 8 n^3 + n^4) + \right.$ 
    n (2 + n) (4 + n) (1 + 3 n + n2) (-1)n +
    (-2 (1 + n) (2 + n) (3 + n) + 2 (1 + n) (2 + n)2 (3 + n)
    (-1)n)  $\sum_{\ell_1=0}^n \frac{-3 + (2 \ell_1 + 3 \ell_1^2 + \ell_1^3) (-1)^{\ell_1}}{1 + \ell_1}$ 
 $\left. \right) \}$  }
```

• *Solving the recurrence with Harmonic numbers*

```
SigmaReduce  $\left[ \sum_{\ell_1=0}^n \frac{-3 + (2 \ell_1 + 3 \ell_1^2 + \ell_1^3) (-1)^{\ell_1}}{1 + \ell_1}, \right.$ 
  SimpleSumRepresentation -> True]
```

$$\frac{1}{2} \left(-1 + (1 + 3 n + n^2) (-1)^n - 6 \sum_{\ell_1=0}^n \frac{1}{1 + \ell_1} \right)$$

```
recSol2 = SolveRecurrence[rec2,
  SUM[n], Tower -> {Hn}, WithMinusPower -> True]
```

```
{ {0, -n (2 + n) (4 + n) + (9 + 28 n + 23 n2 + 8 n3 + n4) (-1)n },
  {0, -(2 + n) (-57 + 16 n + 4 n2) +
    (-21 + 112 n + 92 n2 + 32 n3 + 4 n4) (-1)n }, {1,
   $\frac{1}{76} (-n (650 + 630 n + 143 n^2) + 152 (1 + n) (2 + n) (3 + n) H_n +$ 
    (-195 + 1040 n + 1845 n2 + 916 n3 + 143 n4 -
    152 (1 + n) (2 + n)2 (3 + n) Hn) (-1)n } }
```

• Finding the linear combination

```
solution2 = FindLinearCombination[recSol2, mySum2, 2] //
SigmaSimplify
```

$$-(3+n)(-1+3n+2n^2) + 2(1+n)(2+n)(3+n)H_n + \\ ((3+n)(-1+6n+7n^2+2n^3) - 2(1+n)(2+n)^2(3+n)H_n) \\ (-1)^n$$

▼ Sum1+Sum2



```
solution1 + solution2 / ((n + 1) (n + 2) (n + 3)) //
SigmaSimplify
```

$$-2 + (2+n)(-1)^n$$

For all $n \geq 1$ we have:

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



Finding Sum Extensions (C.S.):

- Inspired by Abramov/Petkovsek and Hendrik/Singer

sum extensions \subset Liouvillian extensions

- Generalization to the $\Pi\Sigma$ -differencefield setting

Ismail, Stanton

Tribasic integrals and identities of Rogers–Ramanujantype

$$\sum_{j=0}^n \left((-1)^{\frac{1}{2}j(1+j)} \left(\prod_{i=1}^j q^n \right) \left(\frac{1}{q^n}, q \right)_j \cdot (1 - q (q^j)^2) \right) /$$

$$\left((q^2 q^n, q)_j \cdot (1 - q) \right) =$$

$$\frac{(-1, q^2)_n \cdot (q^2, q)_n}{(-q, q)_n \cdot (q, q^2)_n}$$

$$\text{mySum} = \sum_{j=0}^n \frac{\left(\frac{(-1)^{\frac{1}{2}j(1+j)} \left(\prod_{i=1}^j q^n \right) \left(\frac{1}{q^n}, q \right)_j}{(q^2 q^n, q)_j} \right)_j \cdot (1 - q (q^j)^2)}{1 - q};$$

```
rec = GenerateRecurrence[
  mySum, Tower -> {{SigmaPower[q, n], n}},
  WithMinusPower -> True]
```

Order: 1

Solution!

$$\{-(-1 + q^2 q^n) (1 + (q^n)^2) \text{SUM}[n] +$$

$$(-1 - q q^n + q (q^n)^2 + q^2 (q^n)^3) \text{SUM}[1 + n] == 0\}$$

A Simple Example

Find a closed form for

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

$$\text{mySum} = \sum_{k=1}^n H_k \binom{n}{k};$$

```
rec = GenerateRecurrence[mySum]
```

```
Order: 1
```

```
Order: 2
```

```
Solution!
```

$$\{4(1+n) \text{SUM}[n] - 2(3+2n) \text{SUM}[1+n] + (2+n) \text{SUM}[2+n] == 1\}$$

```
recSol = SolveRecurrence[rec[[1]],  
SUM[n], Tower -> {2^n}, NestedSumExt -> Infinity]
```

$$\left\{ \{0, 2^n\}, \left\{0, 2^n \sum_{\ell_1=1}^n \frac{1}{\ell_1}\right\}, \left\{1, -2^n \sum_{\ell_1=1}^n \frac{1}{\ell_1 2^{\ell_1}}\right\} \right\}$$

```
FindLinearCombination[recSol, mySum, 2]
```

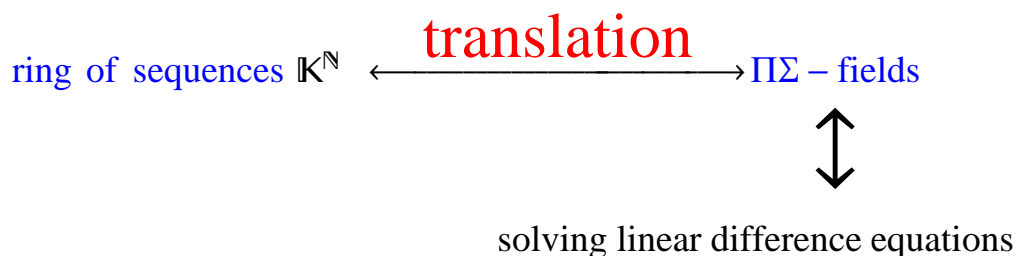
$$2^n \sum_{\ell_1=1}^n \frac{1}{\ell_1} - 2^n \sum_{\ell_1=1}^n \frac{1}{\ell_1 2^{\ell_1}}$$



GOAL: show

$$\sum_{k=1}^n H_k \binom{n}{k} = H_n 2^n + -2^n \sum_{k=1}^n \frac{1}{k 2^k}, \quad n \geq 1$$

in human readable style.



This **translation** needs many notations and is very subtle (poles)

⇒ *Work just in $\mathbb{K}^{\mathbb{N}}$!*



Z's Creative Telescoping Trick

GIVEN:

$$\text{SUM}[n] := \sum_{k=1}^n \underbrace{\left(H_k \binom{n}{k} \right)}_{f[n, k]}$$

Find: $c_0[n]$, $c_1[n]$, $c_2[n]$ and $g[n, k]$ such that

$$g[n, k+1] - g[n, k] = c_0[n] f[n, k] + c_1[n] f[n+1, k] + c_2[n] f[n+2, k]$$

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

Summing this equation over k from 1 to n gives

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

PART II: Proving Sum Identities

<< **Theorema**

Theorema provides various facets of proving, solving and simplifying in *human readable fashion*.

Needs ["Theorema" Provers "UserProvers" SigmaProver"]

Sigma - A summation package by Carsten
Schneider - © RISC Linz - V 1.01 β (12 / 06 / 02)

The Binomial and Harmonic Numbers

Proposition["BinomialHarmonic",

$$\forall_{n \geq 1} \left(\sum_{k=1, \dots, n} \left(H_k * \binom{n}{k} \right) = \left(2^n * H_n - 2^n * \sum_{k=1, \dots, n} \left(\frac{1}{k * 2^k} \right) \right) \right)$$

Prove[Proposition["BinomialHarmonic"], by → **SigmaProver**]

Order: 1

Order: 2

Solution!

- ProofObject -



[WebPage](#)

[LaTeX](#)

PART III: Discovering and Proving

INPUT:

$$\text{FindClosedForm} \left[\sum_{i=1, \dots, n} \left(H_i \binom{n}{i} \right) \right]$$

RESULT:

Proposition["NEW PROPOSITION",

$$\forall_{n \geq 1} \left(\sum_{i=1, \dots, n} \left(H_i \binom{n}{i} \right) = 2^n H_n - 2^n \sum_{i=1, \dots, n} \left(\frac{1}{i 2^i} \right) \right)$$

plus proof.