

Implementation of an Algorithm on Converting Sums into Nested Sums

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Joint Work with Carsten Schneider of RISC



Outlines

- 1 Background & Motivation
 - A Quick Introduction on Nested Sums
 - Sigma.m Package of RISC
- 2 The Algorithm [C. Anzai & Y. Sumino]
 - Steps of the Algorithm
 - Problems.
- 3 Conclusion

Nested Sums

Definition

An indefinite nested sum usually has the form

$$\begin{aligned}
 S(\nu) &= \sum_{\wedge(\nu) \geq j_1 \geq j_2 \geq \dots \geq j_n \geq 1} f_1(j_1) f_2(j_2) \dots f_n(j_n). \\
 &= \sum_{j_1=1}^{\wedge(\nu)} f_1(j_1) \sum_{j_2=1}^{j_1} f_2(j_2) \dots f_{n-1}(j_{n-1}) \sum_{j_n=1}^{j_{n-1}} f_n(j_n)
 \end{aligned}$$

Example

$$\sum_{j_1=0}^m \sum_{j_2=0}^{j_1} \dots \sum_{j_n=0}^{j_{n-1}} 1 = \binom{m+n}{n}$$

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Nested Sums Continued

Examples

$$\left\{ \begin{array}{l} Z(n; m_1, \dots, m_k; x_1, \dots, x_k) := \sum_{n \geq i_1 > \dots > i_k > 0} \frac{x_1^{i_1}}{i_1^{m_1}} \dots \frac{x_k^{i_k}}{i_k^{m_k}} \quad \text{Z-sum} \\ S(n; m_1, \dots, m_k; x_1, \dots, x_k) := \sum_{n \geq i_1 \geq \dots \geq i_k \geq 1} \frac{x_1^{i_1}}{i_1^{m_1}} \dots \frac{x_k^{i_k}}{i_k^{m_k}} \quad \text{S-sum} \\ H(n; a_1, \dots, a_k) := \sum_{n \geq i_1 \geq \dots \geq i_k \geq 1} \frac{\text{sign}(a_1)^{i_1}}{i_1^{|a_1|}} \dots \frac{\text{sign}(a_k)^{i_k}}{i_k^{|a_k|}} \quad \text{H-sum} \end{array} \right.$$

Remark

$$Z(\infty; s; 1) = S(\infty; s; 1) = \sum_{i=1}^{\infty} \frac{1}{i^s} = \zeta(s)$$

$$H(n; 1) = \sum_{i=1}^n \frac{1}{i} = H_n; \quad H(n; p (> 0)) = \sum_{i=1}^n \frac{1}{i^p}$$

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Why “Nested” Sums

$$S_1(\nu) := \sum_{x=1}^{\nu} \frac{1}{(x + \nu)^2}$$

$$S_2(\nu) := \sum_{x=0}^{\nu-1} \left[\frac{1}{(1+2x)^2} + \underbrace{\frac{1}{(2+2x)^2} - \frac{1}{(1+x)^2}}_{=-\frac{3}{4(1+x)^2}} \right]$$

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Convergence.

Example

$$S(\infty) = \sum_{i_1=1}^{\infty} \frac{\sum_{i_2=1}^{i_1} \frac{\sum_{i_3=1}^{i_2} \dots}{i_2^{m_2}}}{i_1^{m_1}}.$$

Theorem

S(∞) is convergent iff $m_1 > 1$ [provided that $S(\infty)$ has only finitely many sums].

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Reason III for Choosing Nested Sums

“Algebraic Relations to Reduce the Sum”.

Remark

This is what the “Sigma.m” package does. [A mathematica package that Carsten works on for years to deal with “all”(at least hypergeometric) sums/products]

Algebraic Relations

In short, given a nested sum, we want to express it in terms of known special functions, e.g. S-sums, Z-sums, ${}_A F_B$, etc. Algebraic relations could help us to find the minimal basis for the expression and reduce the sum.

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Sigma.m Package

“Sigma is a Mathematica package that can handle multisums in terms of indefinite nested sums and products. The summation principles of Sigma are: telescoping, creative telescoping and recurrence solving. The underlying machinery of Sigma is based on difference field theory. The package has been developed by Carsten Schneider, a member of the RISC Combinatorics group. “

“The source code for this package is password protected. To get the password send an email to Peter Paule. It will be given for free to all researchers and non-commercial users.

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<http://www.risc.jku.at/research/combinat/software/Sigma/index.php>

Sigma.m Package (Continued)

In short, “Sigma.m” deals with general multisums.

The algorithm I am working on deals with special case.

Form of the Required Sums

$$S(\nu) = \sum_{i_1=a_1(\nu)}^{b_1(\nu)} \sum_{i_2=a_2(\nu, i_1)}^{b_2(\nu, i_1)} \cdots \sum_{i_n=a_n(\nu, i_1, \dots, i_{n-1})}^{b_n(\nu, i_1, \dots, i_{n-1})} \frac{\lambda_1^{i_1} \cdots \lambda_n^{i_n}}{\prod_r L_r(\nu, i_1, \dots, i_n)^{p_r}},$$

where

$$\begin{cases} \lambda_k \in \mathbb{C} \\ p_k \in \mathbb{N} = \{1, 2, \dots\} \\ L_r \text{ is a linear polynomial with integer coefficients} \\ a_k, b_k \text{ are either infinity or linear polynomials with integer coefficients} \end{cases}$$

NOTE: The number of products in the denominator is unknown.

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$$\sum_{k=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{(k+m)^2(2m+4k+1)} = 4 - 2\mathcal{C}\pi - \frac{\pi^2}{6} - 4 \log 2 + \frac{21}{4}\zeta(3).$$

$$\sum_{k=1}^{\infty} \sum_{m=1}^k \frac{(-1)^{k+m}}{(k+1)^2(2m+1)} = 8\text{Im} [Z(\infty; 2, 1; -i, i)] + 4\mathcal{C} \log 2 - \frac{\pi^3}{8} - \frac{\pi^2}{12}.$$

Where, $\mathcal{C} = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2}$ —Catalan Constant

An Important Notation

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$$\sum_{k=a}^b f(k) = \begin{cases} \sum_{k=a}^b f(k) & a \leq b \\ 0 & a = b + 1. \\ - \sum_{k=b+1}^{a-1} f(k) & a \geq b + 2 \end{cases}$$

Example

$$\sum_{x=5}^2 x = - \sum_{x=3}^4 x = -7$$

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Key Idea—Invariant under Shifting

Find a set of integers $(\Delta_0, \Delta_1, \dots, \Delta_n)$, s.t.

- (1) $\Delta_0 \neq 0$
- (2) $\forall r,$

$$L_r(\nu + \Delta_0, i_1 + \Delta_1, \dots, i_n + \Delta_n) = L_r(\nu, i_1, \dots, i_n).$$

[Question] Does such an integer vector always exist?

[Answer] No. For example, when the number of L_r 's is larger than the number of sums.

Example

$$S(\nu) = \sum_{m=0}^{\infty} \frac{1}{(\nu + m)^2 (4\nu + 2m + 1)}.$$

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Step I——Partial Fraction Decomposition(PFD)

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KEY: From the Innermost Sum Index to the Outermost

Example

$$\sum_{x \geq y \geq z} \frac{1}{(x+y)(y+z)(x+z)} = \sum_{x \geq y \geq z} \frac{1}{2x} \left[\frac{1}{x+y} + \frac{1}{x-y} \right] \left[\frac{1}{y+z} - \frac{1}{x+z} \right].$$

Result

For each part of the sum, the number of L_r 's is **NO GREATER THAN** the number of sums, i.e. it guarantees the existence of the invariant shifting vector $(\Delta_0, \Delta_1, \dots, \Delta_n)$.

NOTE

The solution $(\Delta_0, \Delta_1, \dots, \Delta_n)$ has at least one free variable to turn rational solutions into integer solutions.

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Step II—Key Step (Idea)

For a (not completely known) function $f(x)$, suppose we want to compute $f(101)$, by knowing the following

$$\begin{cases} f(2) \\ \Delta f(x) := f(x+3) - f(x) \end{cases} .$$

Noting that

$$101 \equiv 2 \pmod{3}$$

$$\begin{aligned} f(101) &= f(98) + [f(101) - f(98)] \\ &= f(98) + \Delta f(98) \\ &= \dots \\ &= f(2) + \sum_{k=0}^{32} \Delta f(3k+2) . \end{aligned}$$

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$$S(\nu) = \sum_{i_1=a_1(\nu)}^{b_1(\nu)} \sum_{i_2=a_2(\nu, i_1)}^{b_2(\nu, i_1)} \cdots \sum_{i_n=a_n(\nu, i_1, \dots, i_{n-1})}^{b_n(\nu, i_1, \dots, i_{n-1})} \frac{\lambda_1^{i_1} \cdots \lambda_n^{i_n}}{\prod_{r=1}^n L_r(\nu, i_1, \dots, i_n)^{p_r}},$$

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and

$$\Delta S(\nu) := S(\nu + \Delta_0) - \lambda S(\nu).$$

Step II—Key Step(Continued)

Define

$$\begin{cases} \alpha_k := a_k(\nu + \Delta_0, i_1 + \Delta_1, \dots, i_{k-1} + \Delta_{k-1}) - a_k(\nu, i_1, \dots, i_{k-1}) \in \mathbb{Z} \\ \beta_k := b_k(\nu + \Delta_0, i_1 + \Delta_1, \dots, i_{k-1} + \Delta_{k-1}) - b_k(\nu, i_1, \dots, i_{k-1}) \in \mathbb{Z} \end{cases}.$$

Then

$$\begin{aligned} S(\nu + \Delta_0) &= \sum_{i_1=a_1(\nu+\Delta_0)}^{b_1(\nu+\Delta_0)} \cdots \sum_{i_n=a_n(\nu+\Delta_0, i_1, \dots, i_{n-1})}^{b_n(\nu+\Delta_0, i_1, \dots, i_{n-1})} \frac{\lambda_1^{i_1} \cdots \lambda_n^{i_n}}{\prod_{r=1}^n L_r(\nu + \Delta_0, i_1, \dots, i_n)^{p_r}} \\ [i_k \mapsto i_k + \Delta_k] &= \sum_{i_1+\Delta_1=a_1+\alpha_1}^{b_1+\beta_1} \cdots \sum_{i_n+\Delta_n=a_n+\alpha_n}^{b_n+\beta_n} \frac{\lambda_1^{i_1+\Delta_1} \cdots \lambda_n^{i_n+\Delta_n}}{\prod_{r=1}^n L_r(\nu + \Delta_0, i_1 + \Delta_1, \dots, i_n + \Delta_n)^{p_r}} \\ &= \lambda \underbrace{\sum_{i_1=a_1+\alpha_1-\Delta_1}^{b_1+\beta_1-\Delta_1} \cdots \sum_{i_n=a_n+\alpha_n-\Delta_n}^{b_n+\beta_n-\Delta_n} \frac{\lambda_1^{i_1} \cdots \lambda_n^{i_n}}{\prod_{r=1}^n L_r(\nu + \Delta_0, i_1, \dots, i_n)^{p_r}}}_{su:=}. \end{aligned}$$

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Step II—Key Step(Continued)

$$\begin{aligned} \Delta S(\nu) &= S(\nu + \Delta_0) - \lambda S(\nu) \\ &= \lambda \left[\sum_{i_1=a_1+\alpha_1-\Delta_1}^{b_1+\beta_1-\Delta_1} \cdots \sum_{i_n=a_n+\alpha_n-\Delta_n}^{b_n+\beta_n-\Delta_n} - \sum_{i_1=a_1}^{b_1} \cdots \sum_{i_n=a_n}^{b_n} \right] SU \end{aligned}$$

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$\Delta S(\nu)$ has at least one quantifier less. Thus, by induction, it can be converted into nested sum

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$$\begin{aligned} \Delta S(\nu) &= S(\nu + \Delta_0) - \lambda S(\nu) \\ &= \lambda \left[\sum_{i_1=a_1+\alpha_1-\Delta_1}^{b_1+\beta_1-\Delta_1} \cdots \sum_{i_n=a_n+\alpha_n-\Delta_n}^{b_n+\beta_n-\Delta_n} - \sum_{i_1=a_1}^{b_1} \cdots \sum_{i_n=a_n}^{b_n} \right] SU \end{aligned}$$

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Step II—Key Step(Continued)

Recall:

$$f(101) = f(2) + \sum_{k=0}^{32} \Delta f(3k+2).$$

Define

$$\text{Proj}(m, n, d) = \frac{1}{d} \sum_{k=1}^d \exp\left(2\pi i k \frac{m-n}{d}\right) = \begin{cases} 0 & m \not\equiv n \pmod{d} \\ 1 & m \equiv n \pmod{d} \end{cases}.$$

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[Question] How to deal with $S(\nu_0)$?

FACT(Good News)

$$\nu_0 \in \{0, 1, \dots, \Delta_0\} \implies S(\nu_0) \text{ is determined.}$$

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Example

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$$\begin{aligned}
 S(\nu) &= \sum_{x=1}^{\nu} \sum_{y=1}^x \frac{1}{(\nu - x + 1)(x + y + 1)} \\
 &= \sum_{x=0}^{\nu-1} \frac{1}{3(1+x)} + \sum_{x=0}^{\nu-1} \sum_{y=0}^{x-1} \frac{1}{2(x+2)} \left[\frac{1}{y+1} - \frac{1}{y+2} \right] \\
 &\quad - \sum_{x=0}^{\nu-1} \sum_{y=0}^{x-1} \frac{1}{x+3} \left[\frac{1}{y+1} + \frac{1}{y+3} \right] \\
 &\quad + \sum_{x=0}^{\nu-1} \sum_{y=0}^{x-1} \frac{1}{2x+5} \left[\frac{1}{y+1} + \frac{1}{2y+5} \right]
 \end{aligned}$$

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Speed.

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Problem I — Compatibility with Sigma.m

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Sigma.m can only deal with the cases when the upper bound of the inner sum is the index of the next outer sum.

$$\dots f_{k+1}(i_{k+1}) \sum_{i_k=1}^{i_{k+1}} f_k(i_k) \dots \checkmark$$

$$\dots f_{k+1}(i_{k+1}) \sum_{i_k=1}^{i_{k+1}-1} f_k(i_k) \dots \times$$

Solution

Shift the sum index, ACCORDINGLY.

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Problem II—Root of Unity

Recall:

$$\text{Proj}(m, n, d) = \frac{1}{d} \sum_{k=1}^d \exp\left(2\pi i k \frac{m-n}{d}\right) = \begin{cases} 0 & m \not\equiv n \pmod{d} \\ 1 & m \equiv n \pmod{d} \end{cases}$$

Example

$$\begin{cases} \text{Proj}(m, n, 1) \equiv 1 \\ \text{Proj}(m, n, 2) = \frac{(-1)^m + (-1)^n}{2} \end{cases}$$

When $d \geq 3$, root of unity is inevitable.

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$$\text{Proj}(6, 2, 3) = \frac{1}{3} \left(1 + e^{-\frac{2\pi i}{3}} + e^{\frac{2\pi i}{3}}\right) = 0$$

Mathematica

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Mathematica

Problem II—Root of Unity

Recall:

$$\text{Proj}(m, n, d) = \frac{1}{d} \sum_{k=1}^d \exp\left(2\pi i k \frac{m-n}{d}\right) = \begin{cases} 0 & m \not\equiv n \pmod{d} \\ 1 & m \equiv n \pmod{d} \end{cases}.$$

Example

$$\begin{cases} \text{Proj}(m, n, 1) \equiv 1 \\ \text{Proj}(m, n, 2) = \frac{(-1)^m + (-1)^n}{2} \end{cases}$$

When $d \geq 3$, root of unity is inevitable.

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Problem II—Root of Unity (Continued)

FACT

There is no other substitutions for the projector function.

Solutions/Compromise

- 1 Try to make Δ_0 as small as possible. ($\Delta_0 = 1$ or $\Delta_0 = 2$)
- 2 “Replacement $\nu \mapsto \Delta_0\nu$ ”. (Conditionally)

We can only make such replacement for the outermost sum.

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Problem III—Poles

FACT

It is very common when converting sums into nested sums.

Example

[Created by PFD]

$$S(\nu) = \sum_{x=1}^{\nu} \frac{1}{(\nu+x)(x+1)} \Rightarrow S(1) = \frac{1}{4}$$

$$\begin{aligned} \bar{S}(\nu) &= \sum_{x=1}^{\nu} \left[\frac{1}{(\nu-1)(\nu+x)} - \frac{1}{(\nu-1)(x+1)} \right] \\ &= \frac{1}{\nu-1} \sum_{x=0}^{\nu-1} \left[\frac{1}{x+2} + \frac{1}{x+1} - \frac{1}{2x+1} - \frac{1}{2x+2} \right] \\ \bar{S}(1) &= \frac{0}{0} = \text{"Indetermined"} \end{aligned}$$

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Problem III—Poles (Continued)

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[Created by Shifting (Crossing the Boundary)]

$$S(\nu) = \sum_{x=1}^{\nu} \sum_{z=1}^{x-1} \frac{1}{(\nu+x+1)(x+z)}.$$

Note:

$$\Delta_0 = 1, \Delta_x = \Delta_1 = -1, \Delta_z = \Delta_2 = 1.$$

Fact

While computing $\Delta S(\nu)$, the following sum appears

$$\sum_{x=1}^{\nu} \sum_{z=(x-1)+1}^{(x-1)+(-1)-1} \frac{1}{(\nu+x+1)(x+z)} = - \sum_{x=1}^{\nu} \left[\frac{1}{(\nu+x+1)(2x-1)} + \frac{1}{(\nu+x+1)(2x-2)} \right],$$

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Dealing with Poles—by Authors

Remark

In the paper, during Step II, when poles/divergence terms are created, they introduce regularization parameter, by $i_k \mapsto i_k + \delta_k$. Also, the paper talks about Step III, evaluation, which one can eventually send $\delta_k \rightarrow 0$.

Example

$$\sum_{x \geq y \geq z \geq 1} \frac{1}{2x(x-y)(x+z)} \mapsto \sum_{x \geq y \geq z \geq 1} \frac{1}{2x(x-y+\delta)(x+z)}$$

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The speed will be slowed down dramatically by introducing more parameters, which violates our original purpose for implementation.

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Dealing with Poles—Modifying the Starting Point

[Q]: Recall the expression

$$S(\nu) = \lambda^{\frac{\nu}{\Delta_0}} \sum_{\mu_0=0}^{\Delta_0-1} \text{Proj}(\nu, \mu_0, \Delta_0) \left[\lambda^{-\frac{\mu_0}{\Delta_0}} S(\mu_0) + \sum_{\mu=0}^{\nu-1} \text{Proj}(\mu, \mu_0, \Delta_0) \Delta S(\mu) \lambda^{-\frac{\mu+\Delta_0}{\Delta_0}} \right],$$

and suppose $\Delta S(\mu)$ has a pole at $\mu = 1$. How to deal with it?

RECALL

$$\begin{aligned} f(101) &= f(2) + \sum_{k=0}^{32} \Delta f(3k+2) \\ &= f(5) + \sum_{k=1}^{32} \Delta f(3k+2) \\ &= \dots \end{aligned}$$

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KEY

Find $k \in \mathbb{N}$, s.t. $k \cdot \Delta_0 > 1$ (the largest pole of $\Delta S(\mu)$ & $S(\nu_0)$).

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- 1 This algorithm works faster than the usual/general method of Sigma.m.
- 2 Root of unity is inherited from the algorithm. It seems to be impossible to avoid.
- 3 Poles are very common while converting sums (creating telescoping). And the poles created by PFD is easier to deal with comparing to those from shifting.
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Thank you!