Computer Proofs of a New Family of Harmonic Number Identities

Scott Ahlgren [1]

Department of Mathematics
University of Illinois
Urbana, IL 61801, USA
`ahlgren@math.uiuc.edu`

Peter Paule

Research Institute for Symbolic Computation
Johannes Kepler University Linz
A–4040 Linz, Austria
`Peter.Paule@risc.uni-linz.ac.at`

Carsten Schneider [2]

Research Institute for Symbolic Computation
Johannes Kepler University Linz
A–4040 Linz, Austria
`Carsten.Schneider@risc.uni-linz.ac.at`

Abstract

In this paper we consider five conjectured harmonic number identities similar to those arising in the context of supercongruences for Apéry numbers. The general object of this article is to discuss the possibility of automating not only the proof but also the discovery of such formulas. As a specific application we consider two different algorithmic methods to derive and to prove the five conjectured identities. One is based on an extension of Karr's summation algorithm in difference fields. The other method combines an old idea of Newton (which has been extended by Andrews) with Zeilberger's algorithm for definite hypergeometric sums.

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1 Introduction

For a positive integer n let $\mathrm{H}_n = 1 + \frac{1}{2} + \cdots + \frac{1}{n}$ denote the nth harmonic number. It will be convenient to define $\mathrm{H}_n = 0$ whenever n is non-positive. The object of this paper is the discussion of two new algorithmic approaches which are used to prove the following family of identities for $n \geq 1$:

$$\sum_{j=0}^{n}(1 - j\,\mathrm{H}_j + j\,\mathrm{H}_{n-j})\binom{n}{j} = 1, \tag{1}$$

$$\sum_{j=0}^{n}(1 - 2\,j\,\mathrm{H}_j + 2\,j\,\mathrm{H}_{n-j})\binom{n}{j}^2 = 0, \tag{2}$$

$$\sum_{j=0}^{n}(1 - 3\,j\,\mathrm{H}_j + 3\,j\,\mathrm{H}_{n-j})\binom{n}{j}^3 = (-1)^n, \tag{3}$$

$$\sum_{j=0}^{n}(1 - 4\,j\,\mathrm{H}_j + 4\,j\,\mathrm{H}_{n-j})\binom{n}{j}^4 = (-1)^n\binom{2\,n}{n}, \tag{4}$$

$$\sum_{j=0}^{n}(1 - 5\,j\,\mathrm{H}_j + 5\,j\,\mathrm{H}_{n-j})\binom{n}{j}^5 = (-1)^n\sum_{j=0}^{n}\binom{n}{j}^2\binom{n+j}{j}. \tag{5}$$

It will be convenient to rewrite the left sides of these identities in the form

$$R_n^{(\alpha)} + S_n^{(\alpha)} \tag{6}$$

where for $\alpha \in \{1, \ldots, 5\}$,

$$R_n^{(\alpha)} = \sum_{j=0}^{n}\binom{n}{j}^\alpha \quad \text{and} \quad S_n^{(\alpha)} = \alpha\sum_{j=0}^{n}(n-2j)\mathrm{H}_j\binom{n}{j}^\alpha. \tag{7}$$

Binomial sums like that on the right side of (5) play a crucial role in Apéry's approach to prove the irrationality of $\zeta(2)$ and $\zeta(3)$; see, for instance, the informal report [vdP79]. In an attempt to prove certain 'supercongruences' for Apéry numbers which were conjectured by Beukers, certain harmonic number identities popped up in [AO00,Ah02] (see also the recent works of Mortenson [Mor02a,Mor02b]). In particular, these formulas arise out of computations involving the p-adic gamma function. This motivated S. Ahlgren to do a heuristic search in order to explore whether there are more harmonic number identities of a similar form. The result of this study was a family of *conjectured* identities, namely (1)–(5) above.

Until recently there has been no algorithm to derive *definite* summation identities involving harmonic numbers. For example, the solution to 'bonus problem 69' [GKP94, Chapt. 6],"Find a closed form for $\sum_{k=1}^{n} k^2 \, \mathrm{H}_{n+k}$", ends with the remark, "It would be nice to automate the derivation of formulas such as this". This situation changed due to work [Sch02a,Sch02b,Sch02c,Sch02d] of one of the authors which extends Karr's *indefinite* summation algorithm [Kar81,Kar85] (Karr's algorithm is based on the theory of difference fields [Coh65]). Schneider extends Karr's method to *definite* summation and to solving linear difference equations with polynomial coefficients not only of first but of arbitrary order. These developments have been implemented in the form of the Mathematica package *Sigma* [Sch00], which we have used in all of our computations for the examples below.

Remark. Our emphasis in this article is on the problem of automating the *derivation* of such formulas as (1)–(5). Concerning computer assistance in *proving* such formulas there are other recent methods; see, e.g., Chyzak's generalization of the Gosper-Zeilberger algorithm [CS98] or Wegschaider's package *Multisum* [Weg97] for simplifying multiple hypergeometric sums.

In Section 3 we will demonstrate how identities such as (1)–(5) can be proved — and found — with the *Sigma* package. We want to emphasize that the underlying algebraic theory is quite complex but also very general. As a consequence, the scope of applications of *Sigma* is much broader. Besides hyper- and q-hypergeometric sums which could also involve harmonic numbers and their q-analogues, it can also handle summation problems built by multiple nested sums of very general kind [Sch01]. Therefore it is natural to ask whether there is a more elementary algorithmic approach for proving identities like (1)–(5).

It turns out that this is indeed the case. In Section 2 we introduce a new algorithmic approach to prove definite harmonic number identities such as (1)–(5). The two building blocks of this approach are well-known. Its algorithmic ingredient is Zeilberger's algorithm [Zei90,PWZ96] which is implemented in all major computer algebra systems. This is combined with an operator method for rewriting harmonic numbers in terms of binomial coefficients which, as explained below, traces back to Newton.

In Section 4 we compare the methods of Section 2 and Section 3, and draw some conclusions.

2 An Algorithmic Version of the Newton-Andrews Method

Let L be the operator which evaluates functions $f(x)$ at $x = 0$, i.e., $L\,f(x) := f(0)$. Let D be differentiation with respect to x, i.e., $D\,f(x) := f'(x)$. It is an easy exercise to verify that for all integers n,

$$LD\binom{x+n}{n} = \mathrm{H}_n. \tag{8}$$

This crucial observation in many cases allows us to handle harmonic number identities by reducing them to a hypergeometric problem, a technique often used by G.E. Andrews in his work. In [AU85] one finds the following statement: "Richard Askey has pointed out to us that indeed Issac Newton was the first to see that the partial sums of the harmonic series arise from differentiation of a product [N60, p. 561]."

We illustrate the method by an elementary example, namely $S(n) := \sum_{j=0}^{n} \mathrm{H}_j$, $n \geq 0$. Using (8) and then the hypergeometric summation identity [GKP94, (5.9)]

$$\sum_{j=0}^{n} \binom{x+j}{j} = \left(1 + \frac{n}{1+x}\right)\binom{x+n}{n}, \tag{9}$$

the given sum becomes

$$S(n) = LD\sum_{j=0}^{n} \binom{x+j}{j} = LD\left(1 + \frac{n}{1+x}\right)\binom{x+n}{n}. \tag{10}$$

By applying the product rule for differentiation this simplifies further to

$$S(n) = \mathrm{H}_n + L\left(-\frac{n}{(1+x)^2}\right)\cdot L\binom{x+n}{n} + L\left(\frac{n}{1+x}\right)\cdot \mathrm{H}_n = \mathrm{H}_n - n + n\,\mathrm{H}_n, \tag{11}$$

which in turn becomes the well-known fact [GKP94, (6.67)]

$$\sum_{j=0}^{n} \mathrm{H}_j = (n+1)\,\mathrm{H}_n - n, \qquad n \geq 0. \tag{12}$$

In this particular example the given sum as well as the underlying hypergeometric summation (9) are indefinite, but obviously the method extends also to the definite case. However, applying the method in this classical fashion will always lead to the problem of simplifying the hypergeometric sums which arise. Hence, from algorithmic point of view, it is a natural step to link the Newton-Andrews method with Zeilberger's paradigm of 'creative telescoping'. How such a combination is turned into an effective algorithm becomes transparent in the proof of identity (1).

Proof of Identity (1)**.** It is convenient to prove (1) in the equivalent form

$$\sum_{j=0}^{n} (n-2j)\,\mathrm{H}_j \binom{n}{j} = 1 - 2^n, \qquad n \geq 0, \tag{13}$$

which is obtained from (1) by geometric summation and by reversing the order of summation in the sum $\sum_{j=0}^{n} j\,\mathrm{H}_{n-j}\binom{n}{j}$. The left side of (13) is nothing but $S_n^{(1)}$, and we obtain from (8) that

$$S_n^{(1)} = LD\,t_n(x) \quad \text{where} \quad t_n(x) := \sum_{j=0}^{n}(n-2j)\binom{x+j}{j}\binom{n}{j}. \tag{14}$$

Applying Zeilberger's algorithm (we used *Sigma*) returns the recurrence relation

$$2(n+1)\,t_n(x) - (x+3n+3)\,t_{n+1}(x) + (n+1)\,t_{n+2}(x) = 0, \qquad n \geq 0. \tag{15}$$

The next step is to apply the differentiation operator D to both sides of (15) which results in the mixed differential-difference equation

$$2(n{+}1)\,t_n'(x) - t_{n+1}(x) - (x{+}3n{+}3)\,t_{n+1}'(x) + (n{+}1)\,t_{n+2}'(x) = 0, \quad n \geq 0. \tag{16}$$

Finally we apply the operator L to both sides of (16) which gives

$$2(n+1)\,S_n^{(1)} - (3n+3)\,S_{n+1}^{(1)} + (n+1)\,S_{n+2}^{(1)} = t_{n+1}(0), \quad n \geq 0. \tag{17}$$

Now it is an elementary fact that for all $n \geq 0$,

$$t_n(0) = \sum_{j=0}^{n}(n-2j)\binom{n}{j} = 0, \tag{18}$$

which can be also found by Gosper's algorithm [Gos78]. Therefore, in order to find the right side of (13) one only needs to solve

$$2\,S_n^{(1)} - 3\,S_{n+1}^{(1)} + S_{n+2}^{(1)} = 0, \quad n \geq 0, \tag{19}$$

with initial conditions $S_0^{(1)} = 0$ and $S_1^{(1)} = -1$, which again can be done algorithmically. $\square$

2.1 The Newton-Andrews-Zeilberger Algorithm

Before summarizing in the form of an algorithm description, we recall that S_n is a hypergeometric sequence if there exists a rational function $r(x)$ such that $S_{n+1}/S_n = r(n)$ for all sufficiently large n. Similarly, a term $f(n,j)$ is called hypergeometric in n and j, if the quotients $f(n+1,j)/f(n,j)$ and $f(n,j+1)/f(n,j)$ are rational functions in n and j.

Newton-Andrews-Zeilberger Algorithm. *Input:* a term $f(n,j)$ which is hypergeometric in n and j; *Output:* a linear recurrence of type (22) or (24), respectively, for the sum S_n of the form

$$S_n := \sum_j \mathrm{H}_j f(n,j) \quad \text{or} \quad S_n := \sum_j f(n,j)/\mathrm{H}_j, \quad \text{respectively.} \tag{20}$$

The algorithm can be applied if Zeilberger's algorithm succeeds in finding a recurrence for the sum $t_n(x)$ of the form

$$t_n(x) := \sum_{j=0}^{n} \binom{x+j}{j} f(n,j) \quad \text{or} \quad t_n(x) := \sum_{j=0}^{n} \binom{x+j}{j}^{-1} f(n,j), \text{ respectively.} \tag{21}$$

By (8) we have that $S_n = LD\, t_n(x)$. Consequently, by applying to the $t_n(x)$-recurrence successively the operators D and L (as described in the proof of identity (1)), a recurrence for S_n can be derived in the form

$$a_d(n)\, S_{n+d} + a_{d-1}(n)\, S_{n+d-1} + \cdots + a_0(n)\, S_n = \sum_{i=0}^{d} p_i(n) t_{n+i}(0), \tag{22}$$

where the $a_l(n)$ and $p_i(n)$ are polynomials in n, and where $a_d(n)$ is non-zero.

In addition, by Zeilberger's algorithm and by difference equation solvers like [Pet92] and [vH99] we can decide algorithmically (see also [A02]) whether

$$t_n(0) = \sum_{j=0}^{n} f(n,j) \tag{23}$$

is a hypergeometric sequence in n. If so, each $t_{n+i}(0)$ is a rational function multiple of $t_n(0)$ and therefore also $\sigma_n := \sum_{i=0}^{d} p_i(n) t_{n+i}(0)$. Consequently, the recurrence (22) simplifies to

$$a_d(n)\, S_{n+d} + a_{d-1}(n)\, S_{n+d-1} + \cdots + a_0(n)\, S_n = \sigma_n, \tag{24}$$

where σ_n is a hypergeometric sequence in n.

Applications. Suppose the Newton-Andrews-Zeilberger algorithm outputs a recurrence of the form (24). Then difference equation solvers like [Pet92] and [vH99] can be used to decide algorithmically whether S_n finds a closed form representation as a linear combination of hypergeometric terms. But even if S_n does not find a closed form representation as a linear combination of hypergeometric terms, it might happen that for a given sequence R_n the sequence $R_n + S_n$ does have such a representation, which is the case for the identities (3) and (4); see below.

In general, suppose a linear recurrence for R_n is available in the form

$$b_e(n)\, R_{n+e} + b_{e-1}(n)\, R_{n+e-1} + \cdots + b_0(n)\, R_n = \tau_n \tag{25}$$

where τ_n is a hypergeometric sequence and the $b_l(n)$ are polynomials in n, and $b_e(n)$ is non-zero. Then using procedures from the packages [SZ94] or [Mal96], the recurrences (22) and (24) can be combined into a single homogeneous linear recurrence

$$c_h(n)\, T_{n+h} + c_{h-1}(n)\, T_{n+h-1} + \cdots + c_0(n)\, T_n = 0 \tag{26}$$

where the $c_l(n)$ are polynomials in n with $c_h(n)$ non-zero, which is satisfied by the sequence $T_n := R_n + S_n$. Finally by applying difference equation solvers like [Pet92] or [vH99] one finds a closed form representation of $R_n + S_n$ as a linear combination of hypergeometric terms.

In principle, there are possibilities to extend the Newton-Andrews-Zeilberger algorithm to the case where the summand of S_n involves products (or quotients of products) of harmonic numbers, but then one has to consider many extra conditions. Nevertheless, such methods could contribute to possible extensions of computer algebra packages that rely only on Zeilberger's algorithm. Due to the fact that Schneider's extension of Karr's work described in Section 3 covers all these applications in a natural way, we refrain from presenting further details. Only for comparing the two methods, we give short versions of the Newton-Andrews-Zeilberger derivations of (2)–(4). Concerning identity (5), we emphasize the well-known fact that its right side is not expressible as a hypergeometric term in n, so the Newton-Andrews-Zeilberger algorithm cannot derive this representation. However for the sake of completeness we will briefly describe how a variation of this method can be used to *prove* identity (5).

2.2 Newton-Andrews-Zeilberger Proofs of (2)–(5)

Proof of Identity (2)**.** We use the well-known Vandermonde evaluation $\sum_j \binom{n}{j}^2 = \binom{2n}{n}$ to rewrite (2) in the form

$$\sum_{j=0}^{n} (n-2j)\, \mathrm{H}_j \binom{n}{j}^2 = -\frac{1}{2}\binom{2n}{n}, \qquad n \geq 1. \tag{27}$$

The rewrite rule (8) gives that

$$S_n^{(2)} = LD\, t_n(x) \quad \text{where} \quad t_n(x) := \sum_{j=0}^{n} (n-2j) \binom{x+j}{j} \binom{n}{j}^2, \tag{28}$$

and the Newton-Andrews-Zeilberger algorithm applied as in the proof of identity (1) leads to the recurrence relation

$$
\begin{aligned}
2n(2n+1)(3n+5)\, S_n^{(2)} - (n+1)(15n^2+31n+12)\, S_{n+1}^{(2)} \\
+ (n+1)(n+2)(3n+2)\, S_{n+2}^{(2)} \\
= (3n+5)(4n+1)t_n(0) + (6n^2+13n+4)t_{n+1}(0), \quad n \geq 1. \quad (29)
\end{aligned}
$$

Now it is an elementary fact that for all $n \geq 0$,

$$
t_n(0) = \sum_{j=0}^{n} (n-2j) \binom{n}{j}^2 = 0, \tag{30}
$$

which can be also found by Gosper's algorithm [Gos78]. Therefore, in order to find the right side of (27) one only needs to solve

$$
\begin{aligned}
2n(2n+1)(3n+5)\, S_n^{(2)} - (n+1)(15n^2+31n+12)\, S_{n+1}^{(2)} \\
+ (n+1)(n+2)(3n+2)\, S_{n+2}^{(2)} = 0, \quad n \geq 1, \quad (31)
\end{aligned}
$$

with initial conditions $S_1^{(2)} = -1$ and $S_2^{(2)} = -3$, which again can be done algorithmically by applying difference equation solvers like [Pet92] or [vH99].

□

Next we present the

Proof of Identity (3)**.** According to (6), identity (3) is of the form

$$
R_n^{(3)} + S_n^{(3)} = (-1)^n. \tag{32}
$$

Now $R_n^{(3)}$ does not have a representation as a hypergeometric term since the Zeilberger output recurrence for $R_n^{(3)}$ is

$$
(n+2)^2\, R_{n+2}^{(3)} - (7n^2+21n+16)\, R_{n+1}^{(3)} - 8(n+1)^2\, R_n^{(3)} = 0, \tag{33}
$$

which does not have any hypergeometric solution. Nevertheless, since the right side of (32) is hypergeometric, we can apply the Newton-Andrews-Zeilberger algorithm to find this evaluation. With this procedure we find

$$
\begin{aligned}
& 8(1+n)^3(2+n)^2 \left(1281 + 1245n + 398n^2 + 42n^3\right) S_n^{(3)} \\
& + (1+n)\,(2+n)^2 \left(3600 + 19701n + 25952n^2 + 13953n^3 + 3332n^4 + 294n^5\right) S_{n+1}^{(3)} \\
& - (1+n) \times \big(367440 + 995280n + 1138190n^2 + 714313n^3 \\
& \qquad + 266290n^4 + 59081n^5 + 7236n^6 + 378n^7\big) S_{n+2}^{(3)} \\
& - (1+n)\,(3+n)^2 \left(31600 + 65268n + 52370n^2 + 20491n^3 + 3920n^4 + 294n^5\right) S_{n+3}^{(3)} \\
& + (1+n)\,(3+n)^2(4+n)^2 \left(392 + 575n + 272n^2 + 42n^3\right) S_{n+4}^{(3)} = 0 \quad (34)
\end{aligned}
$$

as the recurrence for $S_n^{(3)}$. As described above, we apply the package *GeneratingFunctions.m* with input (33) and (34) to obtain the recurrence

$$
\begin{aligned}
&8(1+n)^2(2+n)^2(1281+1245n+398n^2+42n^3)S_n^{(3)}\\
&\quad+(2+n)^2(3600+19701n+25952n^2+13953n^3+3332n^4+294n^5)S_{n+1}^{(3)}\\
&\quad+(-367440-995280n-1138190n^2-714313n^3\\
&\qquad\qquad-266290n^4-59081n^5-7236n^6-378n^7)S_{n+2}^{(3)}\\
&\quad-(3+n)^2(31600+65268n+52370n^2+20491n^3+3920n^4+294n^5)S_{n+3}^{(3)}\\
&\qquad\qquad+(3+n)^2(4+n)^2(392+575n+272n^2+42n^3)S_{n+4}^{(3)}=0 \qquad (35)
\end{aligned}
$$

for $T_n := R_n^{(3)} + S_n^{(3)}$. Finally with the solvers [Pet92] or [vH99] one finds that $T_n = (-1)^n$, which completes the proof of (3). □

Proof of Identity (4) — **Sketch.** According to (6), identity (4) is of the form

$$R_n^{(4)} + S_n^{(4)} = (-1)^n \binom{2n}{n}. \qquad (36)$$

Again, $R_n^{(4)}$ does not have a representation as a hypergeometric term, so one proceeds completely analogously to the proof of (3). We refrain from giving the details; however, we mention the fact that despite obtaining again an order 4 recurrence for $T_n := R_n^{(4)} + S_n^{(4)}$, the integer coefficients of the polynomials involved become quite large. □

Using the Newton-Andrews-Zeilberger algorithm, not only can we prove the identities (1)– (4), but we can also *find* the corresponding closed forms on their right sides. With the last identity the situation is slightly different.

Proof of Identity (5)—**Sketch.** According to (6), identity (5) is of the form

$$R_n^{(5)} + S_n^{(5)} = A_n \qquad (37)$$

where

$$A_n = (-1)^n \sum_{j=0}^{n} \binom{n}{j}^2 \binom{n+j}{j} \qquad (38)$$

is a sequence of Apéry numbers. Again Zeilberger's algorithm and the Newton-Andrews-Zeilberger algorithm deliver a recurrence for $R_n^{(5)}$ and $S_n^{(5)}$, respectively. As described above, from these recurrences one obtains a homogeneous linear recurrence for $T_n := R_n^{(5)} + S_n^{(5)}$ which turns out to be of order 6 (and big enough to fill one page). But this time the right side A_n is a definite sum which does not simplify to a hypergeometric term, so we are not able to *find* A_n as the solution to this recurrence since there is no algorithm available for this task so far. However, the task of *proving* identity (5) can be completed algorithmically, for instance, as follows. With Zeilberger's algorithm compute the recurrence

$$(n+2)^2\, A_{n+2} - (11n^2 + 33n + 25)\, A_{n+1} - (n+1)^2\, A_n = 0. \qquad (39)$$

Then using procedures from the packages [SZ94] or [Mal96] with input (39) and the Newton-Andrews-Zeilberger recurrence for $T_n := R_n^{(5)} + S_n^{(5)}$, one computes a homogeneous linear recurrence for $Q_n := R_n^{(5)} + S_n^{(5)} - A_n$ which turns out to be of order 6. Finally, checking that $Q_i = 0$ for i from 1 to 6 completes the proof of (5). $\square$

3 Sigma: A Summation Package for Discovering and Proving

Karr developed an algorithm for indefinite summation [Kar81,Kar85] based on the theory of difference fields [Coh65]. He introduced so called $\Pi\Sigma$-fields in which first order linear difference equations can be solved in full generality. This algorithm deals not only with sums over hypergeometric terms, like Gosper's algorithm [Gos78,PP95], or over q-hypergeometric terms, like [PR97], but also with summations over terms in which, for example, the harmonic numbers can appear in the denominator. Generally speaking, Karr's algorithm is the summation counterpart of Risch's algorithm [Ris70] for indefinite integration.

Inspired by this algorithm, Schneider developed a significantly more general algorithmic summation theory [Bro00,Sch02a,Sch02b,Sch02c,Sch02d] also based on difference field theory. In addition, Schneider implemented his algorithms in the computer algebra system Mathematica. The corresponding summation package *Sigma* also provides a user interface that dispenses the user from working explicitly with difference fields. Instead, the user can handle all summation problems conveniently in terms of usual sum and product expressions; see [Sch00,Sch01].

An important aspect of Schneider's work is his extension of Karr's original method in such a way that *definite* summation problems can be treated too. For example, in [Sch02a] it is shown how the definite summation identity

$$\sum_{j=0}^{n} \mathrm{H}_j \binom{n}{j} = 2^n\, \mathrm{H}_n - 2^n \sum_{j=1}^{n} \frac{1}{j\, 2^j}, \qquad n \geq 0. \qquad (40)$$

can be derived automatically with the *Sigma* package. Note that identity (40) expresses the first definite summation component $\sum_{j=0}^{n} \mathrm{H}_j \binom{n}{j}$ of $S_n^{(1)}$ as a linear combination of 2^n times the *indefinite* sums H_n and $\sum_{j=1}^{n} \frac{1}{j\, 2^j}$, respectively.

The definite sum $\sum_{j=0}^{n} j\,\mathrm{H}_j\binom{n}{j}$ is the second component of the sum $S_n^{(1)}$. So, before turning to the other $S_n^{(\alpha)}$ we will first demonstrate how one can *derive* for this sum an evaluation similar to (40).

We start the Mathematica session by loading the package with
In[1]:= << **Sigma**‘

`Sigma - A summation package by Carsten Schneider © RISC-Linz`

Then we set up the summation problem as follows:

In[2]:= **mySum =**

$$\mathbf{SigmaSum[j\,SigmaHNumber[j]SigmaBinomial[n,j],\{j,0,n\}]}$$

$$\text{Out[2]=} \sum_{\mathtt{j}=0}^{\mathtt{n}} \mathtt{j}\,\mathtt{H_j}\binom{\mathtt{n}}{\mathtt{j}}.$$

Remark. The basic functions `SigmaSum` and `SigmaProduct` are used to describe all nested sum and product epressions that can be formulated in ΠΣ-fields. To facilitate this task there are numerous other functions available, like `SigmaHNumber`, `SigmaBinomial` or `SigmaPower`. For instance, `SigmaHNumber`[j] produces the jth harmonic number H_j which alternatively could be described by `SigmaSum[1/k,{k,1,j}]`. Additionally, in order to enable the user to define his/her own objects that can be formulated with nested sums and products, various help functions are provided.

In the first step we ask *Sigma* to compute a recurrence that is satisfied by `mySum`:

In[3]:= **rec = GenerateRecurrence[mySum]**

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

This means that SUM[n] $=\sum_{j=0}^{n} j\,\mathrm{H}_j\binom{n}{j}$ (=mySum) satisfies the output recurrence Out[3].

Remark. To compute such recurrences Zeilberger's creative telescoping [Zei90] has been extended from hypergeometric expressions to terms in ΠΣ-fields; for more information see [Sch01].

Secondly, we try to find solutions to this recurrence. In the given situation it turns out that the algorithm does not find any solution in the underlying difference field $\mathbb{F}$ which has been constructed internally by the objects given in the recurrence `rec`. The *Sigma* package is designed in such a way that when it fails to find a solution to a recurrence within a given difference field $\mathbb{F}$, then it also indicates that there is no *sum extension* of $\mathbb{F}$ in which a solution exists. Therefore we try to extend $\mathbb{F}$ by an appropriate *product extension*. Finding such product extensions is assisted by the function `FindProductExtensions` which uses M. Petkovšek's package `Hyper` [Pet92,Pet94,PWZ96]. This package is able to find all *hypergeometric* solutions of linear recurrences such as Out[3] and has to be loaded first.

In[4]:= $<<$ **Hyper`**
In[5]:= **FindProductExtensions[rec[[1]], SUM[n]]**

```
I use M. Petkovsek's package Hyper to find product extensions!
```

Out[5]= $\{\prod_{i=1}^{n} 2\}$

This step was successful: the output tells us that if we extend the given difference field $\mathbb{F}$ by the new element 2^n, then we will find at least one non-trivial solution to Out[3]. But the *Sigma* package can do much more. Namely, with the next function call we can find not only solutions in $\mathbb{F}(2^n)$, but also solutions in **all** difference fields which extend $\mathbb{F}(2^n)$ by nested sums built from the elements of $\mathbb{F}(2^n)$.

In[6]:= **recSol = SolveRecurrence[rec[[1]], SUM[n],**
NestedSumExt → ∞, Tower → {2^n}]

Out[6]= $\{\{0, n\,2^{n}\}, \{0, n\,2^{n} \sum_{\iota_1=2}^{n} \frac{-2+\iota_1}{(-1+\iota_1)\,\iota_1}\}, \{1, n\,2^{n} \sum_{\iota_1=2}^{n} \frac{1}{(-1+\iota_1)\iota_1 2^{\iota_1}}\}\}$

In this example we have succeeded completely; the output describes two linear independent solutions of the homogeneous variation of the recurrence Out[3], namely $n\,2^n$ and $n\,2^n \sum_{\iota_1=2}^{n} \frac{-2+\iota_1}{(-1+\iota_1)\,\iota_1}$, and one particular solution of the inhomogeneous recurrence itself, namely $n\,2^n \sum_{\iota_1=2}^{n} \frac{1}{(-1+\iota_1)\,\iota_1}$.

Remark. These kind of solutions are called d'Alembertian solutions and are introduced in [AP94]; further results can be found in [HS99] and [Sch01].

Finally, the closed form of `mySum` is that linear combination of the homogeneous solutions plus the inhomogeneous solution which has exactly the same initial values as `mySum`. This is also computed automatically:

In[7]:= **result = FindLinearCombination[recSol,**
mySum, 2, MinInitialValue → 1]

Out[7]= $\frac{1}{2} 2^{n} + \frac{1}{2} n\,2^{n} \sum_{\iota_1=2}^{n} \frac{-2+\iota_1}{(-1+\iota_1)\iota_1} + n\,2^{n} \sum_{\iota_1=2}^{n} \frac{1}{(-1+\iota_1)\iota_1\, 2^{\iota_1}}$

Note that we were only able to find this linear combination starting from $n \geq 1$. This closed form evaluation of `mySum` for $n \geq 1$ can be rewritten as follows. Applying partial fraction decomposition to the summands gives

$$\frac{-2+\iota_1}{(-1+\iota_1)\iota_1} = -\frac{1}{-1+\iota_1} + \frac{2}{\iota_1} \quad \text{and} \quad \frac{1}{(-1+\iota_1)\iota_1 2^{\iota_1}} = \frac{1}{(-1+\iota_1)2^{\iota_1}} - \frac{1}{\iota_1 2^{\iota_1}}.$$

This motivates us to simplify Out[7] further by asking *Sigma* for a representation of the expression `result` by the sums H_n and $\sum_{j=1}^{n}\frac{1}{j\,2^j}$. This is done by the following command.

$\mathsf{In}[8]{:=}\ \mathbf{SigmaReduce}\big[\mathbf{result},\mathbf{n},\mathbf{Tower}\to\{\mathbf{H_k},\sum_{j=1}^{n}\frac{1}{j\,2^{j}}\}\big]$

$\mathsf{Out}[8]{=}\ \frac{1}{2}\Big(-1+(1+n\,\mathrm{H}_n)\,2^{n}-n\,2^{n}\sum_{j=1}^{n}\frac{1}{j\,2^{j}}\Big)$

Summarizing, with *Sigma* we found that

$$\sum_{j=0}^{n} j\,\mathrm{H}_j\binom{n}{j}=\frac{1}{2}\Big(-1+2^n\Big(1+n\,\mathrm{H}_n-n\sum_{j=1}^{n}\frac{1}{j\,2^j}\Big)\Big) \tag{41}$$

holds for all $n\geq 1$; by inspection we see that (41) holds for $n=0$ as well.

3.2 Automatic Discovery of (1) *and* (2)

Combining (40) and (41) we obtain

$$\begin{aligned}\sum_{j=0}^{n}(A\,\mathrm{H}_j+B\,j\,\mathrm{H}_j)\binom{n}{j}&=A\sum_{j=0}^{n}\mathrm{H}_j\binom{n}{j}+B\sum_{j=0}^{n}j\,\mathrm{H}_j\binom{n}{j}\\&=\frac{1}{2}\Big(-B+2^n\Big(B+(2\,A+B\,n)\Big(\mathrm{H}_n-\sum_{j=1}^{n}\frac{1}{j\,2^j}\Big)\Big)\Big).\end{aligned}$$

For the specific choice $A=n$ and $B=-2$ this leads us immediately to (13) which, as pointed out above, is equivalent to (1).

Applying *Sigma* as in Section 3.1 we can find automatically the following two identities

$$\sum_{j=0}^{n}\mathrm{H}_j\binom{n}{j}^2=(2\,\mathrm{H}_n-\mathrm{H}_{2\,n})\binom{2n}{n},\qquad n\geq 0, \tag{42}$$

$$\sum_{j=0}^{n}j\,\mathrm{H}_j\binom{n}{j}^2=\frac{1}{4}\,(1+4\,n\,\mathrm{H}_n-2\,n\,\mathrm{H}_{2\,n})\binom{2n}{n},\qquad n\geq 1, \tag{43}$$

which combine to

$$\sum_{j=0}^{n}(A\,\mathrm{H}_j+B\,j\,\mathrm{H}_j)\binom{n}{j}^2=-\frac{1}{4}\,(B-2\,(2\,A-B\,n)\,(2\,\mathrm{H}_n-\mathrm{H}_{2\,n}))\binom{2n}{n}.$$

By choosing $A = n$ and $B = -2$ we obtain (27) which is equivalent to equation (2).

Summarizing, by using the package *Sigma* we not only succeeded in discovering and proving the first two identities of the family (1) to (5), but derived additionally as a by-product the identities (40),(41), (42), and (43).

3.3 Proving and Finding Identities

In the following we consider the identities (3)–(5). We abbreviate their left sides by $T_n^{(\alpha)}$; recalling (6) this means that $T_n^{(\alpha)} := R_n^{(\alpha)} + S_n^{(\alpha)}$ for $\alpha \in \{3, 4, 5\}$. We will use two different approaches; one direct and one more sophisticated. These are described in the two subsections below. For each approach the general strategy will be the same; namely, we first compute recurrences for the given left sides $T_n^{(\alpha)}$.

More precisely, in the first attempt we will compute these recurrences in the classical way; i.e. by creative telescoping as in the previous subsection. In the second attempt we compute recurrences in a more sophisticated manner, namely by introducing additional sum extensions. It is crucial that these extensions can be found automatically and also that these extensions produce recurrences of smaller order than the direct approach. It turns out that for the given identities these smaller orders are even minimal. In addition to proving the identities, this fact enables us to find the right hand sides of (3)–(5) without any further computations.

3.3.1 The Direct Approach

As mentioned above we first compute recurrences for the sums $T_n^{(\alpha)}$ for $\alpha \in \{3, 4, 5\}$.

$\mathsf{In}[9]{:=}\ \mathbf{mySum3} = \sum_{\mathbf{j=0}}^{\mathbf{n}} \left((\mathbf{1 - 3\,j\,H_j + 3\,(-j + n)\,H_j}) \left(\binom{\mathbf{n}}{\mathbf{j}} \right)^{\mathbf{3}} \right);$

$\mathsf{In}[10]{:=}\ \mathbf{rec3} = \mathbf{GenerateRecurrence}[\mathbf{mySum3}]$

$\mathsf{Out}[10]{=}\ \{(-1 - n)\,\mathtt{SUM}[n] + (-3 - 2\,n)\,\mathtt{SUM}[1 + n] + (-2 - n)\,\mathtt{SUM}[2 + n] == 0\}$

$\mathsf{In}[11]{:=}\ \mathbf{mySum4} = \sum_{\mathbf{j=0}}^{\mathbf{n}} \left((\mathbf{1 - 4\,j\,H_j + 4\,(-j + n)\,H_j}) \left(\binom{\mathbf{n}}{\mathbf{j}} \right)^{\mathbf{4}} \right);$

$\mathsf{In}[12]{:=}\ \mathbf{rec4} = \mathbf{GenerateRecurrence}[\mathbf{mySum4}]$

$$\mathsf{Out}[12]{=}\ \left\{4\,(1 + 2\,n)^2\,(11 + 8\,n)\,\mathtt{SUM}[n] + 2\left(29 + 110\,n + 108\,n^2 + 32\,n^3\right) \mathtt{SUM}[1 + n] + (2 + n)^2\,(3 + 8\,n)\,\mathtt{SUM}[2 + n] == 0\right\}$$

In[13]:= $\mathbf{mySum5} = \sum_{\mathbf{j=0}}^{\mathbf{n}} \Big((\mathbf{1} - \mathbf{5\,j\,H_j} + \mathbf{5}\,(-\mathbf{j}+\mathbf{n})\ \mathbf{H_j}) \left(\binom{\mathbf{n}}{\mathbf{j}}^{\cdot} \right)^{\mathbf{5}} \Big);$

In[14]:= $\mathbf{rec5} = \mathbf{GenerateRecurrence[mySum5]}$

Out[14]= $\{(1+\mathtt{n})^3(2+\mathtt{n})(41752 + 59264\mathtt{n} + 31245\mathtt{n}^2 + 7250\mathtt{n}^3 + 625\mathtt{n}^4)\mathtt{SUM[n]} -$
$(2+\mathtt{n})\,(3007560 + 10401664\,\mathtt{n} + 15087509\,\mathtt{n}^2 + 11895816\,\mathtt{n}^3 +$
$5506508\,\mathtt{n}^4 + 1496890\,\mathtt{n}^5 + 221375\,\mathtt{n}^6 + 13750\,\mathtt{n}^7)\ \mathtt{SUM[1+n]} +$
$(66648040 + 240325672\,\mathtt{n} + 372720670\,\mathtt{n}^2 + 325025288\,\mathtt{n}^3 +$
$174496185\,\mathtt{n}^4 + 59121186\,\mathtt{n}^5 + 12356530\,\mathtt{n}^6 + 1457750\,\mathtt{n}^7 +$
$74375\,\mathtt{n}^8)\ \mathtt{SUM[2+n]} + (3+\mathtt{n})\ (6783960 +$
$21058536\,\mathtt{n} + 27279834\,\mathtt{n}^2 + 19134404\,\mathtt{n}^3 + 7861553\,\mathtt{n}^4 +$
$1895640\,\mathtt{n}^5 + 248875\,\mathtt{n}^6 + 13750\,\mathtt{n}^7)\ \mathtt{SUM[3+n]} + (3+\mathtt{n})\ (4+\mathtt{n})^3$
$(7108 + 16024\,\mathtt{n} + 13245\,\mathtt{n}^2 + 4750\,\mathtt{n}^3 + 625\,\mathtt{n}^4)\ \mathtt{SUM[4+n]} == 0\}$

One can easily verify that $(-1)^n$ is a solution of recurrence `rec3` and that $(-1)^n \binom{2n}{n}$ is a solution of `rec4`. Checking initial values of both sequences proves identities (3) and (4). Note that by applying difference equation solvers like [Pet92] and [vH99] one is even able to *find* the closed form solutions $(-1)^n$ and $(-1)^n \binom{2n}{n}$ automatically.

Since the right side of identity (5) is a definite sum, we have to proceed in a slightly different way. Namely, we compute a recurrence that contains all the solutions of `rec5` and the recurrence given in (39). Using one of the packages [SZ94] or [Mal96] it turns out that the resulting recurrence is again `rec5`. Since the right side A_n defined in (38) is a solution of (39), the expression $T_n^{(5)} - A_n$ is a solution of `rec5`. Consequently, checking that the first four initial values of $T_n^{(5)} - A_n$ are 0 implies that $T_n^{(5)} - A_n$ is zero for all $n \geq 1$, which completes the proof of identity (5).

Remark. A different approach would be to combine $T_n^{(5)} - A_n$ into a single definite sum expression and to compute its defining linear recurrence by applying the *Sigma* function call `GenerateRecurrence` to it. Again it turns out that the result is recurrence `rec5`.

We want to emphasize that both strategies only prove identity (5). They do not *find* its right side; this situation will change in the more sophisticated approach of Section 3.2.2. Moreover, we remark that if one applies the *Sigma* function call `GenerateRecurrence` directly to the left side sums in (3)–(5), it turns out that the computations are much more involved and the orders of the resulting recurrences in comparison to the orders of `rec3` to `rec5` are increased by one. This indicates that ‘creative symmetrizing’ introduced for hypergeometric sums in [Pau94] plays an essential role also in the algorithmic treatment of sums where, for instance, harmonic numbers are involved.

3.3.2 A More Sophisticated Approach: Recurrences with Sum Extensions

Schneider's summation theory provides a new mechanism which finds certain sum extensions automatically. The details of this method are described in [Sch01, Section 4.4.3], so we restrict ourselves to brief descriptions of its application to the identities (3)–(5). We shall see that the orders of the recurrences computed by this approach are significantly smaller than those of `rec3` to `rec5`.

Identity (3). For `mySum3` (resp. $T_n^{(3)}$) we are able to find the following recurrence of order 1 instead of order 2 as in Out[10].

In[15]:= **rec3 = GenerateRecurrence[mySum3, SimplifyByExt → DepthNumber]**

$$\text{Out[15]}= \left\{(1+n)\,\mathrm{SUM}[n] + (1+n)\,\mathrm{SUM}[1+n] == 3\left(n - \sum_{\iota_1=1}^{n} \frac{(2+n-2\,\iota_1)\,\iota_1^3\left(\binom{n}{\iota_1}^{\cdot}\right)^3}{(1+n-\iota_1)^3}\right)\right\}$$

In a second step we can show with *Sigma* that the sum on the right side is equal to n for all $n \geq 0$. This shows that $T_n^{(3)}$ satisfies

$$T_n^{(3)} + T_{n+1}^{(3)} = 0$$

which allows us to read off the closed form representation $T_n^{(3)} = (-1)^n$. Obviously this recurrence for $T_n^{(3)}$ is the minimal possible one.

Identity (4). For `mySum4` (resp. $T_n^{(4)}$) we are able to find the following recurrence of order 1 instead of order 2 as in Out[12].

In[16]:= **rec4 = GenerateRecurrence[mySum4, SimplifyByExt → DepthNumber]**

$$\text{Out[16]}= 2\,(1+n)\,(1+2\,n)\,\mathrm{SUM}[n] + (1+n)^2\,\mathrm{SUM}[1+n] == 2\,(3+8\,n)\left(n - \sum_{\iota_1=1}^{n} \frac{(2+n-2\,\iota_1)\,\iota_1^4\left(\binom{n}{\iota_1}^{\cdot}\right)^4}{(1+n-\iota_1)^4}\right)\}$$

In a second step we show with *Sigma* that the right side is equal to 0 for all $n \geq 0$. This proves that $T_n^{(4)}$ satisfies the recurrence

$$2\,(1+2\,n)\,T_n^{(4)} + (1+n)\,T_{n+1}^{(4)} = 0;$$

identity (4) is a direct consequence of this result. In particular, this recurrence has minimal order for $(-1)^n\binom{2n}{n}$, therefore it is also the minimal recurrence for $T_n^{(4)}$.

Identity (5). Finally, for `mySum5` (resp. $T_n^{(5)}$), we find the following recurrence of order 2 instead of order 4 as in Out[14].

In[17]:= **rec5 = GenerateRecurrence[mySum5, SimplifyByExt → DepthNumber]**

$$\text{Out[17]= } \Big\{ -(1+n)^2(2+n)\,\mathrm{SUM}[n]+ (2+n)\left(25+33n+11n^2\right)\mathrm{SUM}[1+n]+(2+n)^3\,\mathrm{SUM}[2+n]== n(1+n)\left(-340-690n-255n^2+525n^3+681n^4+319n^5+55n^6\right)+ (1+n)(13+10n)\sum_{\iota_1=0}^{n}\frac{(2+n-2\iota_1)\,\iota_1^5\left(\binom{n}{\iota_1}\right)^5}{(1+n-\iota_1)^5}- (1+n)^5\left(109+154n+55n^2\right)\sum_{\iota_1=0}^{n}\frac{(3+n-2\iota_1)\,\iota_1^5\left(\binom{n}{\iota_1}\right)^5}{(1+n-\iota_1)^5(2+n-\iota_1)^5}\Big\}$$

In a second step we show with *Sigma* that the right side is equal to 0 for all $n \geq 0$. Therefore we obtain the recurrence

$$-(1+n)^2\,T_n^{(5)}+\left(25+33\,n+11\,n^2\right)T_{n+1}^{(5)}+(2+n)^2\,T_{n+2}^{(5)}=0$$

for all $n \geq 0$. Observing that this is, up to an alternating sign variation, the well-known recurrence (39) of the Apéry numbers enables us to guess the right side A_n in (5). The guess is verified by checking the first two initial values. Again this recurrence is the minimal possible one for $T_n^{(5)}$. Consequently, by identifying the output recurrence as the Apéry recurrence we have even **found** the right hand side of identity (5).

4 Conclusion

Before we conclude with an open problem we compare the two different approaches of the previous sections.

In the Newton-Andrews-Zeilberger approach, using (8) one sets up a more general hypergeometric summation problem that contains the original harmonic number summation. For this more general problem a Zeilberger recurrence is computed. In order to solve the original harmonic number summation problem, this recurrence is specialized by differentiation and evaluation. The generality of this approach is also its computational bottleneck. More precisely, in many cases this ansatz finds only recurrences with a drastically higher recurrence order than necessary. For instance, for proving identity (5) we have to compute a recurrence of order 6 instead of order 4 as in Out[14] or order 2 as in Out[17].

Moreover, when products or quotients of several harmonic numbers appear in the summand, one has to introduce additional variables in order to translate the problem to the hypergeometric setting which reduces the efficiency of the algorithm tremendously. Additionally, in this case, as pointed out in Section 2, one has to consider many extra conditions. Depending on their complexity, in general there is no guarantee that a desired recurrence for the given definite summation problem can be derived by restricting to hypergeometric tools only. Nevertheless, in practice many problems are of the simple type (20); so the Newton-Andrews-Zeilberger approach could well serve as a useful extension of any implementation of Zeilberger's algorithm.

The approach followed by the *Sigma* package is completely different. Nested sum expressions, including summations involving harmonic numbers, are translated in a natural way into the corresponding difference field setting and, by using a very general algebraic machinery, the problem is solved there. Clearly, if one restricts these general algorithms to the hypergeometric case, they cannot compete in performance with the hypergeometric special purpose provers and solvers. But, due to the richness of the underlying algebraic structure, the *Sigma* approach provides much more flexibility and efficiency when dealing with definite *nested* sum expressions. Here we want to mention that with the *Sigma* package we can go on to compute recurrences for the sums $T_n^{(\alpha)}$ as illustrated in Subsection 3.3.2. For instance, for $\alpha = 6$ and $\alpha = 7$ we obtain recurrences that are quite out of scope for the 'naive' hypergeometric approach, namely

$$\begin{multline}3\,(1+n)\,(2+3\,n)\,(4+3\,n)\,T_n^{(6)}-\\(3+2\,n)\left(30+39\,n+13\,n^2\right)T_{n+1}^{(6)}-(2+n)^3\,T_{n+2}^{(6)}=0 \quad (44)\end{multline}$$

and

$$\begin{multline}-(1+n)^4\left(39+33\,n+7\,n^2\right)T_n^{(7)}-\big(56667+199575\,n+290457\,n^2+\\223446\,n^3+95773\,n^4+21675\,n^5+2023\,n^6\big)\,T_{n+1}^{(7)}+\\\big(29445+89733\,n+111973\,n^2+73282\,n^3+26575\,n^4+5073\,n^5+\\399\,n^6\big)\,T_{n+2}^{(7)}+(3+n)^4\left(13+19\,n+7\,n^2\right)T_{n+3}^{(7)}=0. \quad (45)\end{multline}$$

Using the *Sigma* package, we computed recurrences for $T_n^{(\alpha)}$ up to $\alpha = 9$. Remarkably, for $3 \le \alpha \le 9$, these recurrences are the same as the recurrences we computed with *Sigma* or Zeilberger's algorithm for the hypergeometric sum

$$U_n^{(\alpha)} := \sum_{j=0}^{n}(n-2j)\binom{n}{j}^{\alpha}, \quad (46)$$

also parameterized by α. We do not know whether the Zeilberger recurrences for $U_n^{(\alpha)}$ coincide with the minimal recurrences of the $T_n^{(\alpha)}$ for *all* $\alpha \ge 3$. Note that the sums $T_n^{(\alpha)}$ are highly non-trivial whereas it is easy to prove that the $U_n^{(\alpha)}$ evaluate to zero for all $\alpha, n \ge 0$.

Another open problem is the question of whether the sum $T_n^{(\alpha)}$ for *all* $\alpha \geq 3$ finds a representation in terms of a definite hypergeometric single-sum.

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