PADÉ APPROXIMATIONS TO THE LOGARITHM II: IDENTITIES, RECURRENCES, AND SYMBOLIC COMPUTATION

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Abstract. Combinatorial identities that were needed in [24] are proved, mostly with C. Schneider's computer algebra package *Sigma*. The form of the Padé approximation of the logarithm of arbitrary order is stated as a conjecture.

1. Introduction

In this paper we derive a number of recurrences and combinatorial identities, mostly by symbolic computation and occasionally by hand, all related to the problem of finding Padé approximations to the logarithm based at $x = 1$.

For given positive integers m and n, the problem consists of finding $n+1$ polynomials $r_m(x)$, $s_m(x)$, …, $t_m(x)$, each of degree at most m, such that

$$r_m(x)\big(\log x\big)^n + s_m(x)\big(\log x\big)^{n-1} + \cdots + t_m(x) = O\big((x-1)^{(n+1)(m+1)-1}\big). \tag{1}$$

The case $n = 1$, with m arbitrary, leads to the well-known (m, m) Padé approximation to the logarithm, namely

$$r_m(x)\log(x) + s_m(x) = O\big((x-1)^{2m+1}\big). \tag{2}$$

Likewise, the case $n = 2$ leads to the (m, m, m) Hermite-Padé quadratic approximation

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

where, of course, the $r_m(x)$ and $s_m(x)$ are not the same polynomials as in (2).

The polynomials $r_m(x)$, $s_m(x)$, …, $t_m(x)$, are interesting in that they also appear in certain finite difference formulas, as well as certain inverse Laplace transforms [24]. The computation of these polynomials is therefore important, and both explicit formulas as well as recurrence relations are available, at least for the cases $n = 1, 2, 3$ and 4.

For these values of n, explicit formulas for $r_m(x)$, $s_m(x)$, …, $t_m(x)$ have been derived in [24]. Some of the proofs in [24] are incomplete, however, in that certain combinatorial identities need to be established. These identities are validated in this paper, with the aid of C. Schneider's package for symbolic summation, *Sigma* [20, 18].

Whereas explicit formulas are aesthetic and useful for theoretical purposes, recurrence relations might be more practical for computation. Such recurrences can be found by inspection in the case $n = 1$ (see [24]), and for $n = 2$ they have been derived by P. Borwein [2]. Here

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we derive also the recurrence formulas corresponding to $n = 3$ and $n = 4$, again using the package *Sigma*.

To give an idea of the identities that will be considered in this paper, we quote

$$\sum_{k=0}^{m}\left[\binom{m}{k}^2 + k\frac{d}{dk}\binom{m}{k}^2\right] = 0, \qquad m = 1, 2, 3, \dots, \tag{4}$$

which was obtained in [24]. We shall present several independent proofs of (4) in this paper.

Regarding notation, we express the binomial coefficient in terms of the Gamma function, Γ, which allows one to write

$$\frac{d}{dk}\binom{m}{k}^2 = 2\binom{m}{k}^2\Big[\psi(m-k+1) - \psi(k+1)\Big], \qquad 0 \le k \le m.$$

The Psi function is defined by $\psi = \Gamma'/\Gamma$ and can be connected to the harmonic numbers via

$$\psi(m-k+1) - \psi(k+1) = H_{m-k} - H_k,$$

where

$$H_0 = 0, \qquad H_k = \sum_{\ell=1}^{k}\frac{1}{\ell}, \quad k \ge 1. \tag{5}$$

An equivalent representation of (4), which also appears in [13], is therefore

$$\sum_{k=0}^{m}\Big(1 + 2\,k\,(H_{m-k} - H_k)\Big)\binom{m}{k}^2 = 0. \tag{6}$$

A more concise form of expressing identities such as these is via operator notation: If we let D represent the operator d/dk, then (4) becomes

$$\sum_{k=0}^{m} D\left[k\binom{m}{k}^2\right] = 0.$$

The outline of the paper is as follows: Since the software package *Sigma* is at the center of our investigations, we start with a brief introduction to the mathematics it is based upon, and give an introductory example. In Section 3 we derive the recurrence formulas alluded to above, and in Section 4 we give proofs of several combinatorial identities similar to (6). Further developments are discussed in Section 5, and in Section 6 we present a conjecture about the general form of the polynomials in (1).

In the third part of this series of papers [5] we show how the symbolic computation approach can be enhanced by human reasoning to derive additional combinatorial identities that appear to be new.

2. Automatic proof techniques with *SIGMA*

Until recently there has been no efficient algorithm to derive identities that involve nested definite and indefinite sum expressions, such as (6). This situation changed due to the efforts of one of us [23, 19, 21, 22]. This work, in combination with [3], extends Karr's *indefinite* summation algorithm [10, 11], which is based on the theory of difference fields [4], to *definite* summation and to solving linear difference equations with polynomial coefficients in so-called $\Pi\Sigma$-fields [10] not only of first but of arbitrary order. Karr's original approach cannot only deal with sums over hypergeometric terms, like Gosper's algorithm [6, 14, 15], or over q-hypergeometric terms, like [12], but also with summations over terms in which for example the harmonic numbers can appear in the denominator. Karr's algorithm is, in a sense, the summation counterpart of Risch's algorithm [17] for indefinite integration. Inspired by this algorithm we developed a summation algorithm based on difference field theory that enables one to deal also with definite summation problems. We implemented this algorithm in the computer algebra system Mathematica and developed a user interface that frees 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. The resulting package is called *Sigma* [20, 18].

In this section we wish to illustrate the usage of *Sigma* using the following definite sum identity as model example:

$$\sum_{k=0}^{n}(-1)^{k-1}\binom{n}{k}H_{k+d}=\begin{cases}\dfrac{d!(n-1)!}{(n+d)!} & \text{for } n\geq 1,\\ -H_d & \text{for } n=0.\end{cases} \tag{7}$$

Here d is a positive integer, but in fact the identity remains true for complex values of $d\neq -1,-2,\ldots$, with appropriate interpretation of the symbols.

We shall show how *Sigma* can be used not only to prove the identity (7), but also to discover it. Moreover, we wish to emphasize that afterwards one can verify independently that the identity holds true.

After loading the summation package

In[1]:= << **Sigma`**

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

we set up the summation problem as follows:

In[2]:= **mySum = SigmaSum[**
SigmaPower[−1, k − 1]SigmaBinomial[n, k]SigmaHNumber[k + d], {k, 0, n}]

Out[2]= $\sum_{k=0}^{n}(-1)^{-1+k}\,H_{d+k}\binom{n}{k}$

The functions `SigmaSum` and `SigmaProduct` are used to define nested sums and products that can be formulated in the difference field setting. For this purpose there are also several other functions available, like `SigmaHNumber`, `SigmaBinomial` or `SigmaPower` to define harmonic numbers, binomials or powers in terms of sums and products which itself can be converted into the difference field setting. For instance, `SigmaHNumber[k]` produces the kth harmonic number H_k which alternatively could be described by `SigmaSum[1/i,{i,1,k}]`.

The key strategy to discover the given identity (7) is to compute a recurrence that is satisfied by `mySum`:

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

Out[3]= {−n SUM[n] + (1 + d + n) SUM[1 + n] == 0}

This means that SUM[n] $=\sum_{k=0}^{n}(-1)^{k-1}\binom{n}{k}H_{k+d}$ (= `mySum`) satisfies the output recurrence `rec`. Given this recurrence one can immediately read off the right-hand side of identity (7).

Hence it is immediate that this identity holds if our sum `mySum` is a solution of the computed recurrence `rec`. Therefore the crucial question is how one can verify that this result is really correct. The answer to this question can be given if one looks at how this recurrence has been derived. The basic idea involved in computing and proving correctness is based on Zeilberger's creative telescoping [25] that was originally introduced for hypergeometric series. In *Sigma* algorithms are developed that enable the user to apply this technique not only to hypergeometric terms, but also to a huge class of terms involving an arbitrary number of nested sums and products. In our situation *Sigma* computes for the given two-nested sum

$$\mathrm{SUM}(n,d)=\sum_{k=0}^{n} f(n,d,k)=\sum_{k=0}^{n}(-1)^{k-1}\binom{n}{k}H_{k+d}$$

constants $c_0(n,d), c_1(n,d)$ (independent of k) and an expression $g(n,d,k)$ in terms of harmonic numbers that fulfil a so-called *creative telescoping equation*

$$c_0(n,d)\,f(n,d,k)+c_1(n,d)\,f(n+1,d,k)=g(n,d,k+1)-g(n,d,k) \tag{8}$$

for all $0\le k\le n$, $n\ge 1$ and $d\ge 0$. More precisely, the expressions

$$c_0(n,d)=-n^2,\ c_1(n,d)=n(n+d+1)\ \text{ and }\ g(n,d,k)=\frac{k(k-n-1)+k(d+k)nH_{d+k}}{n+1-k}\binom{n}{k}(-1)^k$$

are computed by

In[4]:= **CreativeTelescoping[mySum]**

$$\text{Out[4]}=\Big\{\{0,0,1\},\Big\{-\mathtt{n}^2,\mathtt{n}\ (1+\mathtt{d}+\mathtt{n}),\frac{(\mathtt{k}\ (-1+\mathtt{k}-\mathtt{n})+\mathtt{k}\ (\mathtt{d}+\mathtt{k})\ \mathtt{n}\ \mathtt{H}_{\mathtt{d}+\mathtt{k}})\binom{\mathtt{n}}{\mathtt{k}}\ (-1)^{\mathtt{k}}}{1-\mathtt{k}+\mathtt{n}}\Big\}\Big\}$$

Now it is essential that one can check independently that this equation (8) holds for all $1\le k\le n$ and all $n\ge 1$ and $d\ge 0$. In the next step one sums the equation (8) over k from 0 to n. This yields

$$c_0(n,d)\sum_{k=0}^{n} f(n,d,k)+c_1(n,d)\sum_{k=0}^{n} f(n+1,d,k)=g(n,d,n+1)-g(n,d,0)$$

by telescoping. Then one can easily check that

$$g(n,d,n+1)-g(n,d,0)+c_1(n,d)\,f(n+1,d,n+1)=0,$$

which immediately delivers the recurrence `rec`.

In the same spirit one can find a closed form evaluation of $T_n:=\sum_{k=1}^{n}\frac{(-1)^{k-1}}{k}\binom{n+d}{k+d}$ which is the inverse relation of the sum $\sum_{k=0}^{n}(-1)^{k-1}\binom{n}{k}H_{k+d}$ given in (7). In particular one can derive a recurrence

$$-n(n+d+1)T_n+n(n+1)T_{n+1}=(d+1)\binom{n+d}{d+1} \tag{9}$$

by applying creative telescoping, as it is described above. On one side, this recurrence can be solved by iteration, which delivers the identity

$$\frac{1}{\binom{n+d}{d}}\sum_{k=1}^{n}\frac{(-1)^{k-1}}{k}\binom{n+d}{k+d}=H_{n+d}-H_d \tag{10}$$

after checking initial values. On the other side, *Sigma* provides several functions to find the right-hand side of this identity by solving the recurrence (9) in terms of d'Alembertian solutions that are introduced in [1]. Further results can be found in [8] and [18].

In general, *Sigma* enables one to find recurrences for a huge class of definite multisums, like for instance `mySum` $= \sum_{k=0}^{n} f(n,k)$, where $f(n,k)$ may consist of nested sum and product expressions. To be more precise, the function call `CreativeTelescoping[mySum]` searches for constants $c_0(n), \dots, c_l(n)$, independent of k, and a sequence $g(n,k)$, such that the creative telescoping equation

$$c_0(n) f_0(n,k) + \cdots + c_l(n) f(n+l,k) = g(n,k+1) - g(n,k)$$

holds for all $1 \le k \le n$, all $n \ge 1$, and some $l \ge 1$. Then, as illustrated above, this not only enables one to compute a recurrence (by telescoping), but also allows one to verify the correctness of the result. Throughout this paper, these ingredients $c_i(n)$ and $g(n,k)$, computed by the function `CreativeTelescoping`, are called the *proof certificate* of `mySum`.

Having introduced some of the basic principles of *Sigma*, we are now ready to apply it to derive recurrences for the polynomials $r_m(x)$, $s_m(x)$, $\dots$, $t_m(x)$ defined in Section 1.

3. Recurrence relations

The leading polynomial, $r_m(x)$, in the Padé approximations (1) can be obtained explicitly for arbitrary m and n, namely [9, 24]

$$r_m(x) = \sum_{k=0}^{m} \binom{m}{k}^{n+1} \Big((-1)^{n+1} x\Big)^k. \tag{11}$$

The other coefficient polynomials, $s_m(x)$, $\dots$, $t_m(x)$, can likewise be obtained explicitly, at least in the cases $n = 1, 2, 3$ and 4; see [24]. These formulas are not as simple as (11), however, and recurrence relations might be preferred for computational purposes. Fortunately, for a given n, the polynomials $s_m(x)$, $\dots$, $t_m(x)$ all satisfy the same recurrence relation as the leading polynomial $r_m(x)$. A proof of this fact is indicated in Theorem 1 of [2], but below we present an independent and different proof. Therefore we need to focus only on the leading polynomial (11) in our quest for finding recurrences.

Such recurrences have been derived for the cases $n = 1$ and $n = 2$ in [24] and [2] respectively. The recurrences for $n = 3$ and $n = 4$, which we believe to be new, are derived below with the aid of computer algebra.

Even though the case $n = 2$ has been considered in [2], we shall re-derive it here with *Sigma* as it is simpler than the cases $n = 3$ and $n = 4$. We quote from [2] that the polynomials $r_m(x)$, $s_m(x)$ and $t_m(x)$, defined in (3), all satisfy the recurrence

$$\begin{aligned}(3m+4)&(m+3)^2 p_{m+3}(x)\\ &= a_m (x-1)^3\, p_m(x) - (b_m x^2 + c_m x + d_m)\, p_{m+1}(x) + e_m (x-1)\, p_{m+2}(x),\end{aligned} \tag{12}$$

for $m \ge 0$, where

$$a_m = (3m+7)(m+1)^2, \qquad b_m = (3m+5)(3m^2+11m+9) = d_m,$$
$$c_m = (3m+5)(21m^2+77m+66), \quad e_m = (9m^3+57m^2+116m+74).$$

Initial values are[1]

$$\begin{aligned} r_0 &= 1, \quad r_1 = x-1, \qquad r_2 = x^2-8x+1,\\ s_0 &= 0, \quad s_1 = -6x-6, \quad s_2 = -9x^2+9,\\ t_0 &= 0, \quad t_1 = 12x-12, \quad t_2 = 24x^2-48x+24. \end{aligned}$$

The *Sigma* verification of (12) proceeds as follows:

$$\text{In[5]:=}\ \mathbf{mySum} = \sum_{\mathbf{k=0}}^{\mathbf{m}} \left(\left(\binom{\mathbf{m}}{\mathbf{k}}\right)^{\mathbf{3}} (-\mathbf{x})^{\mathbf{k}} \right)_{\mathbf{k}};$$

In[6]:= **GenerateRecurrence[mySum]**

```
Out[6]= {(1 + m)^2 (7 + 3 m) (−1 + x)^3 SUM[m] + (5 + 3 m) (11 m (1 + 7 x + x^2) + 3 m^2 (1 + 7 x + x^2)+
        3 (3 + 22 x + 3 x^2)) SUM[1 + m] + (74 + 116 m + 57 m^2 + 9 m^3) (−1 + x) SUM[2 + m]+
         (3 + m)^2 (4 + 3 m) SUM[3 + m] == 0}
```

After collecting the coefficient polynomials in an appropriate way, one concludes that this expression is identical to the recurrence (12).

For completeness we also provide the proof certificate (defined in Section 2), which enables one to set up the creative telescoping equation:

In[7]:= **CreativeTelescoping[mySum]**

```
Out[7]= {{0, 0, 0, 0, 1}, {(1 + m)^2(7 + 3m)(−1 + x)^12, (5 + 3m)(−1 + x)^9
          (11m(1 + 7x + x^2) + 3m^2(1 + 7x + x^2) + 3(3 + 22x + 3x^2)),
        (74 + 116m + 57m^2 + 9m^3)(−1 + x)^10, (3 + m)^2(4 + 3m)(−1 + x)^9,
        (k^3(1 + m)^2(−1 + x)^9(k^6(7 + 3m)(−1 + x)^2 − 3k^5(7 + 3m)(−1 + x)(−6 + 5x + m(−3 + 2x))+
                3k^4(7 + 3m)(47 − 74x + 31x^2 + m^2(12 − 14x + 5x^2) + m(48 − 66x + 25x^2))+
              (2 + m)(3 + m)^2(3m^4(27 + x^2) + 2m^3(297 − 9x + 14x^2) + 2(377 − 87x + 42x^2)+
                  m^2(1587 − 122x + 97x^2) + m(1820 − 262x + 148x^2))−
              3k(3 + m)(2041 − 1041x + 420x^2 + 3m^5(27 − 3x + 2x^2)+
                  m^4(801 − 129x + 71x^2) + 2m^3(1559 − 349x + 167x^2)+
                  m^2(5959 − 1798x + 781x^2) + m(5578 − 2213x + 908x^2))+
              3k^2(3898 − 3372x + 1302x^2 + 3m^5(36 − 12x + 5x^2)+
                  m^4(1143 − 468x + 185x^2) + 4m^3(1192 − 595x + 227x^2)+
                  m^2(9785 − 5912x + 2217x^2) + m(9862 − 7160x + 2693x^2))−
              k^3(4365 − 5408x + 2135x^2+
                  3m^4(81 − 56x + 20x^2) + m^3(2043 − 1652x + 590x^2)+
                  m^2(6359 − 5972x + 2166x^2) + m(8672 − 9392x + 3519x^2)))
          ((Binomial[m, k])^3 (−x)^k)_k ) / ((−3 + k − m)^3(−2 + k − m)^3(−1 + k − m)^3)}}
```

In [2], Borwein stated the fact that $r_m(x)$, $s_m(x)$, and $t_m(x)$ all satisfy the same recurrence without giving details of the proof. Here we give an independent proof based on the methods of the present paper.

[1]Note that there is a typographical error in [2]: the sign of the first term of $t_1(x)$ is incorrect. Note also that the recurrence (12) computes the polynomials with normalization $r_m(0) = (-1)^m$. By contrast, the normalization $r_m(0) = 1$ was employed in [24].

Set $f(m,k) = (-x)^k \binom{m}{k}^3$. Then, by creative telescoping,

$$A_3(m)f(m+3,k) + A_2(m)f(m+2,k) + A_1(m)f(m+1,k) + A_0(m)f(m,k) \\ = g(m,k+1) - g(m,k). \quad (13)$$

Summing on k gives, since the right-hand side is telescoping, the recurrence for $r_m(x)$. However, (13) can be differentiated with respect to k any number of times, and the right-hand side will still be telescoping. Let us discuss the effect of one such differentiation:

$$\sum_{i=0}^{3} A_i(m)(-x)^k \frac{d}{dk}\binom{m+i}{k}^3 + \log(-x)\sum_{i=0}^{3} A_i(m)(-x)^k \binom{m+i}{k}^3 \\ = \frac{d}{dk}g(m,k+1) - \frac{d}{dk}g(m,k).$$

Summing over all k, the right-hand side disappears, as well as the second sum. Consequently,

$$\sum_{i=0}^{3} A_i(m) \sum_k (-x)^k \frac{d}{dk}\binom{m+i}{k}^3 = 0,$$

and so $\sum_k (-x)^k D\binom{m}{k}^3$ satisfies the same recursion as does $\sum_k (-x)^k \binom{m}{k}^3$. This argument can be repeated and thus $\sum_k (-x)^k D^j \binom{m}{k}^3$ satisfies the same recurrence as $r_m(x)$, and any linear combination as well. Although we presented this proof only for the quadratic case, the argument is fully general: Suppose that it is true that each polynomial in the general Padé approximation is a linear combination of $\sum_k ((-1)^{(n-1)}x)^k D^j \binom{m}{k}^n$ (see the conjecture at the end of this paper), then it follows from this discussion that they all satisfy the same recurrence relation.

Finding the recurrences for the $n = 3$ and $n = 4$ cases proceeds analogously, but the results are of course more unwieldy to report. To prevent clutter we do not reproduce the details here, nor the recurrences themselves. Instead, we refer to [**?**].

In contrast to the examples of the previous section, here we are just dealing with terminating definite hypergeometric sums. An alternative approach to deriving these recurrences would therefore be to apply Zeilberger's algorithm [16, 25]. Versions of this algorithm are available for most major computer algebra systems; see for example [14].

4. Identities

In [24], several combinatorial identities were presented. Proofs of some were provided—e.g., identity (4) above—but others were left as conjectures. In this section we present proofs of these conjectures.

In operator notation, $D = d/dk$, the two identities that need to be proved in the quadratic Padé case are (see [24] for details)

$$\sum_{k=0}^{m} (-1)^k \left(D^2 + \pi^2\right) \left[k^\ell \binom{m}{k}^3\right] = 0, \qquad \ell = 0, 1. \quad (14)$$

To prepare these expressions for *Sigma*, they have to be converted to versions that involve harmonic numbers. Owing to the second derivatives with respect to k, the harmonic numbers of the second kind appear, namely

$$H_0^{(2)} = 0, \qquad H_k^{(2)} = \sum_{\ell=1}^{k} \frac{1}{\ell^2}, \quad k \geq 1. \tag{15}$$

The left sides of the identities (14) now become, respectively for $\ell = 0$ and $\ell = 1$,

$$S_m^{(2,0)} := 3\sum_{k=0}^{m}(-1)^k \binom{m}{k}^3 \Big[3(H_{m-k} - H_k)^2 + H_{m-k}^{(2)} + H_k^{(2)}\Big], \tag{16}$$

$$S_m^{(2,1)} := 3\sum_{k=0}^{m}(-1)^k \binom{m}{k}^3 \Big[k(3(H_{m-k} - H_k)^2 + H_{m-k}^{(2)} + H_k^{(2)}) + 2(H_{m-k} - H_k)\Big]. \tag{17}$$

We need to show that these expressions evaluate to 0 for all $m \geq 0$. To simplify, we redefine the quantities $S_m^{(2,0)}$ and $S_m^{(2,1)}$ by omitting the factor 3 in both (16) and (17).

After defining the given definite summation problem $S_m^{(2,0)}$ in *Sigma*

In[8]:= $\mathbf{mySum} = \sum_{\mathbf{k=0}}^{\mathbf{m}} \big(\mathbf{3}\ (\mathbf{H_k} - \mathbf{H_{-k+m}})^{\mathbf{2}} + \mathbf{H_k^{(2)}} + \mathbf{H_{-k+m}^{(2)}}\big)\ \Big(\big(\binom{\mathbf{m}}{\mathbf{k}}\big)^{\mathbf{3}}\ (-\mathbf{1})^{\mathbf{k}}\Big)_{\mathbf{k}}$;

we are capable of computing the following homogeneous recurrence that contains the solution $S_m^{(2,0)} = \mathtt{SUM[m]}(= \mathtt{mySum})$.

In[9]:= **rec = GenerateRecurrence[mySum]**

Out[9]= $\{3\ (2+3\,\mathtt{m})\ (4+3\,\mathtt{m})\ \mathtt{SUM[m]} + (2+\mathtt{m})^2\ \mathtt{SUM}[2+\mathtt{m}] == 0\}$

The proof certificate (defined in Section 2), which enables one to set up the creative telescoping equation, reads as follows:

In[10]:= **CreativeTelescoping[mySum]**

Out[10]=
$$\begin{aligned}
&\{\{0,0,0,1\},\{3(2+3m)(4+3m)(8+3m),0,(2+m)^2(8+3m),\\
&-\Big(k(8+3m)\big(2(1+m)^3\big(2k^6-10k(2+m)^3(3+2m)(8+5m)+10k^2(2+m)^2(5+3m)(8+5m)-\\
&\quad 5k^3(2+m)(8+5m)(9+5m)-k^5(30+17m)+32(29+98m)+k^4(196+m(221+62m))+\\
&\quad 2m^2(2200+m(1640+m(685+2m(76+7m))))\big)+k(-2+k-m)(-1+k-m)\big(3k(-2+k-m)\\
&\quad (-1+k-m)\big(3k^4(4+3m)-3k^3(4+3m)(8+5m)+2(1+m)(2+m)^2(29+2m(20+7m))-\\
&\quad 3k(2+m)(3+2m)(23+m(35+13m))+3k^2(98+m(198+m(132+29m)))\big)\big)H_k^2+\\
&6\big(k^6(4+3m)-4k^5(3+2m)(4+3m)+2(1+m)^2(2+m)^3(29+2m(20+7m))-\\
&\quad 4k(1+m)(2+m)^2(3+2m)(23+m(35+13m))+2k^4(123+m(258+m(179+41m)))-\\
&\quad 2k^3(348+m(971+m(1005+m(457+77m))))+k^2(2+m)(581+m(1737+m(1925+m(937+169m))))\big)H_{-k+m}+\\
&3k(-2+k-m)(-1+k-m)\big(3k^4(4+3m)-3k^3(4+3m)(8+5m)+2(1+m)(2+m)^2(29+2m(20+7m))-\\
&\quad 3k(2+m)(3+2m)(23+m(35+13m))+3k^2(98+m(198+m(132+29m)))\big)H_{-k+m}^2+\\
&6H_k\big(-k^6(4+3m)+4k^5(3+2m)(4+3m)-2(1+m)^2(2+m)^3(29+2m(20+7m))+\\
&\quad 4k(1+m)(2+m)^2(3+2m)(23+m(35+13m))-2k^4(123+m(258+m(179+41m)))+\\
&\quad 2k^3(348+m(971+m(1005+m(457+77m))))-k^2(2+m)(581+m(1737+m(1925+m(937+169m))))-\\
&\quad k(-2+k-m)(-1+k-m)\big(3k^4(4+3m)-3k^3(4+3m)(8+5m)+2(1+m)(2+m)^2(29+2m(20+7m))-\\
&\quad 3k(2+m)(3+2m)(23+m(35+13m))+3k^2(98+m(198+m(132+29m)))\big)H_{-k+m}\big)+\\
&\quad k(-2+k-m)(-1+k-m)\big(3k^4(4+3m)-3k^3(4+3m)(8+5m)+2(1+m)(2+m)^2(29+2m(20+7m))-\\
&\quad 3k(2+m)(3+2m)(23+m(35+13m))+3k^2(98+m(198+m(132+29m)))\big)\big(H_k^{(2)}+H_{-k+m}^{(2)}\big)\big)\Big)\\
&\qquad\Big(\big(\tbinom{m}{k}\big)^3(-1)^k\Big)_k\Big/\big((1-k+m)^5(2-k+m)^5\big)\}\}
\end{aligned}$$

To verify this recurrence, we check that the creative telescoping equation

$$3(3m+2)(3m+4)f(m,k) + (m+2)^2 f(m+2,k) = g(m,k+1) - g(m,k) \tag{18}$$

with

$$f(m,k) := (-1)^k \binom{m}{k}^3 \Big[3(H_{m-k} - H_k)^2 + H^{(2)}_{m-k} + H^{(2)}_k \Big]$$

and $g(m,k)$ computed above (the last component of `Out[10]`) holds for all $0 \le k \le m$ and all $m \ge 0$. Then summing this equation over k from 0 to m, as already described in Section 2, gives us the recurrence `rec`. Since the first two initial values of our sum $S_m^{(2,0)}$ evaluate to zero, it must hold for all $m \ge 0$. In a similar fashion we can compute the recurrence

$$3(3m+1)(3m+2)(6m^2+16m+11)\, S_m^{(2,1)} - 6(3m^2+6m+2)\, S_{m+1}^{(2,1)} \\ + (m+1)(m+2)(6m^2+4m+1)\, S_{m+2}^{(2,1)} = 0 \quad (19)$$

for the sum $S_m^{(2,1)}$ given in (17). Again, with creative telescoping one can verify that this recurrence (19) holds for all $m \ge 0$; the ingredients to set up this creative telescoping equation can be found in [**?**]. Since the sum $S_m^{(2,1)}$ evaluates to 0 for the first two initial values, identity $S_m^{(2,1)} = 0$ follows. Altogether we have proven that identities (14) hold.

Next, we will prove identities that correspond to the case $n = 3$; they are

$$\sum_{k=0}^{m} D(D^2 + 4\pi^2) \left[k^\ell \binom{m}{k}^4 \right] = 0, \qquad \ell = 0, 1, 2. \quad (20)$$

As before we can convert these three identities into a form that involves harmonic numbers, this time introducing also $H_k^{(3)}$ analogous to (5) and (15). Akin to (16) and (17), we end up with three sums that need to be proven identically zero, namely

$$S_m^{(3,0)} := \sum_{k=0}^{m} h(k) \binom{m}{k}^4,$$

$$S_m^{(3,1)} := \sum_{k=0}^{m} \big(3g(k) + 2kh(k)\big) \binom{m}{k}^4$$

and

$$S_m^{(3,2)} := \sum_{k=0}^{m} \big(k^2 h(k) + 3kg(k) + 3f(k)\big) \binom{m}{k}^4$$

Here we have defined, for simplicity,

$$\begin{aligned} f(k) &:= H_{m-k} - H_k, \\ g(k) &:= 4(H_{m-k} - H_k)^2 + H^{(2)}_{m-k} + H^{(2)}_k, \\ h(k) &:= 8(H_{m-k} - H_k)^3 + 6(H_{m-k} - H_k)(H^{(2)}_{m-k} + H^{(2)}_k) + H^{(3)}_{m-k} - H^{(3)}_k. \end{aligned}$$

To prove that $S_m^{(3,0)} = 0$ for all $m \ge 0$, note that $h(m-k) = -h(k)$ and hence

$$S_m^{(3,0)} = \sum_{k=0}^{m} h(k) \binom{m}{k}^4 = \sum_{k=0}^{m} h(m-k) \binom{m}{m-k}^4 = -\sum_{k=0}^{m} h(k) \binom{m}{k}^4 = -S_m^{(3,0)}$$

which proves the first identity. To show that $S_m^{(3,1)}=0$ for all $m\geq 0$, we use *Sigma* to compute the recurrence

$$\begin{aligned}&-8\,(1+m)\,(1+2m)\,(3+4m)\,(5+4m)\left(129+193m+94m^2+15m^3\right)\,S_m^{(3,1)}\\&\quad-4\left(7560+39369m+82597m^2+92434m^3+60256m^4+23024m^5+4792m^6+420m^7\right)\,S_{m+1}^{(3,1)}\\&\quad\quad-2\,(2+m)\left(1425+6187m+9949m^2+7891m^3+3314m^4+706m^5+60m^6\right)\,S_{m+2}^{(3,1)}\\&\quad\quad\quad+(2+m)^2(3+m)^2\left(15+50m+49m^2+15m^3\right)\,S_{m+3}^{(3,1)}=0.\end{aligned}$$

Note that this result can be verified independently by checking that the corresponding creative telescoping equation holds; this proof certificate can be obtained in [**?**]. Since the first three initial values are zero, it follows also that $S_m^{(3,1)}=0$ for all $m\geq 0$.

Finally, we show that the identity $S_m^{(3,2)}=0$ holds for all integers $m\geq 0$. Clearly we have

$$\sum_{k=0}^{m} f(k)\binom{m}{k}^4=0 \tag{21}$$

by splitting the sum and changing the summation order. Applying $h(m-k)=-h(k)$ again, it follows that

$$\begin{aligned}\sum_{k=0}^{m} k^2h(k)\binom{m}{k}^4&=\sum_{k=0}^{m}(m-k)^2h(m-k)\binom{m}{m-k}^4\\&=-\sum_{k=0}^{m}(m^2-2mk+k^2)h(k)\binom{m}{k}^4.\end{aligned}$$

Hence

$$2\sum_{k=0} k^2h(k)\binom{m}{k}^4=-m^2\sum_{k=0}^{m} h(k)\binom{m}{k}^4+2\sum_{k=0}^{m} mkh(k)\binom{m}{k}^4,$$

and therefore since $S_m^{(3,0)}=0$ we conclude that

$$\sum_{k=0}^{m} k^2h(k)\binom{m}{k}^4=\sum_{k=0}^{m} mkh(k)\binom{m}{k}^4 \tag{22}$$

for all $m\geq 0$. Similarly one can show that

$$\sum_{k=0}^{m} kg(k)\binom{m}{k}^4=\sum_{k=0}^{m}\frac{m}{2}g(k)\binom{m}{k}^4 \tag{23}$$

for all $m\geq 0$. By (21), (22) and (23) we obtain

$$S_m^{(3,2)}=\frac{m}{2}\sum_{k=0}^{m}\big(2kh(k)+3g(k)\big)\binom{m}{k}^4=\frac{m}{2}S_m^{(3,1)}=0.$$

To conclude this section, we consider identities that correspond to the case $n=4$, namely

$$\sum_{k=0}^{m}(-1)^k\left(D^2+\pi^2\right)\left(D^2+9\pi^2\right)\left[k^\ell\binom{m}{k}^5\right]=0,\qquad \ell=0,1,2,3. \tag{24}$$

As for the previous cases $n = 2, 3$, these four identities can be rephrased in terms involving harmonic numbers. Introducing $H_k^{(4)}$ analogous to (5) and (15), the first two identities $\ell = 0, 1$ can be rewritten as

$$S_m^{(4,0)} := 5 \sum_{k=0}^{m} (-1)^k \binom{m}{k}^5 \Big[125\big(H_k - H_{m-k}^{(1)}\big)^4 + 150\big(H_k - H_{m-k}^{(1)}\big)^2 \big(H_k^{(2)} + H_{m-k}^{(2)}\big) + 15\big(H_k^{(2)} + H_{m-k}^{(2)}\big)^2 \\ + 40\big(H_k - H_{m-k}\big)\big(H_k^{(3)} - H_{m-k}^{(3)}\big) + 6H_k^{(4)} + 6H_{m-k}^{(4)} \Big]$$

and

$$S_m^{(4,1)} := 5 \sum_{k=0}^{m} (-1)^k \binom{m}{k}^5 \Big[-60\big(H_k - H_{m-k}\big)\big(H_k^{(2)} + H_{m-k}^{(2)}\big) + 4\big(25\big(-H_k + H_{m-k}\big)^3 - 2H_k^{(3)} + 2H_{m-k}^{(3)}\big) \\ + 5k\big(-H_k + H_{m-k}\big)\big(25\big(-H_k + H_{m-k}\big)^3 - 8H_k^{(3)} + 8H_{m-k}^{(3)}\big) \\ + 3k\big(5\big(H_k^{(2)} + H_{m-k}^{(2)}\big)\big(10\big(H_k - H_{m-k}\big)^2 + H_k^{(2)} + H_{m-k}^{(2)}\big) + 2\big(H_k^{(4)} + H_{m-k}^{(4)}\big)\big) \Big].$$

Whereas the first two identities $S_m^{(4,0)} = 0$ and $S_m^{(4,1)} = 0$ illustrate fascinating algebraic relations between the harmonic numbers and still have reasonable size, the last two identities $S_m^{(4,2)} = 0$ and $S_m^{(4,3)} = 0$ each fill more than one page. Thus we decided not to include them here, but rather give them in [**?**]. For all four sums $S_m^{(4,\ell)}$, $\ell = 0, 1, 2, 3$, we computed homogeneous recurrences of order at most four; these results are likewise displayed in [**?**]. Checking that the first four initial values are zero finally proves that $S_m^{(4,\ell)} = 0$ and hence the identities (24).

5. Further identities

In this section we provide several proofs of the following result, which was conjectured in the previous paper [24].

Theorem 1. *For all* $\ell = 0,\ 1,\ 2,\ \dots,\ 2m$,

$$\sum_{k=0}^{m} \frac{d}{dk} \left[k^\ell \binom{m}{k}^2 \right] = 0. \tag{25}$$

Let us start with the case $\ell = 1$, since $\ell = 0$ is trivial

$$\sum_{k=0}^{m} \binom{m}{k}^2 + \sum_{k=0}^{m} k \frac{d}{dk} \binom{m}{k}^2 = 0.$$

Since the first sum is, by Vandermonde's convolution, $\binom{2m}{m}$, we must compute the second sum:

$$\begin{aligned} S := \sum_{k=0}^{m} k \frac{d}{dk} \binom{m}{k}^2 &= \sum_{k=1}^{m} 2k \binom{m}{k}^2 \big(H_{m-k} - H_k\big) \\ &= 2m \sum_{k=1}^{m} \binom{m}{k} \binom{m-1}{k-1} \big(H_{m-k} - H_k\big). \end{aligned}$$

Now we use for natural numbers n, r (compare [7, p. 354])

$$T_{n,r}=\sum_{s=0}^{r-1}\frac{1}{r-s}\binom{s}{n}=\binom{r}{n}\big(H_r-H_n\big).$$

With this notation, we can continue:

$$\begin{aligned}
S&=2m\sum_{k=0}^{m-1}\binom{m}{k+1}\binom{m-1}{k}\Big[\big(H_m-H_{k+1}\big)-\big(H_m-H_{m-k-1}\big)\Big]\\
&=2m\sum_{k=0}^{m-1}\binom{m-1}{k}\Big[T_{k+1,m}-T_{m-k-1,m}\Big]\\
&=2m\sum_{s=0}^{m-1}\frac{1}{m-s}\bigg[\sum_{k=0}^{m-1}\binom{m-1}{k}\binom{s}{k+1}-\sum_{k=0}^{m-1}\binom{m-1}{k}\binom{s}{m-k-1}\bigg]\\
&=2m\sum_{s=0}^{m-1}\frac{1}{m-s}\bigg[\binom{m+s-1}{m}-\binom{m+s-1}{m-1}\bigg]\\
&=-2\sum_{s=0}^{m-1}\binom{m+s-1}{m-1}=-2\binom{2m-1}{m},
\end{aligned}$$

which gives the desired result.

The next quantity to be computed in this context is when $\ell=2$, namely

$$\sum_{k=0}^{m}k^2\frac{d}{dk}\binom{m}{k}^2=2\sum_{k=0}^{m}k^2\binom{m}{k}^2\big(H_{m-k}-H_k\big),$$

which could be done with the same technique. For a change, we use a different method, based on the formula [7, (6.72)]

$$H_n=\sum_{k=1}^{n}\frac{(-1)^{k-1}}{k}\binom{n}{k}.$$

Then

$$\begin{aligned}
\sum_{k=0}^{m}\binom{m}{k}^2k^2(H_{m-k}-H_k)&=\sum_{k=0}^{m}\binom{m}{k}^2\Big((m-k)^2-k^2\Big)H_k\\
&=\sum_{j\ge1}\frac{(-1)^{j-1}}{j}\binom{m}{j}\sum_{k\ge j}\binom{m}{k}\binom{m-j}{k-j}\Big((m-k)^2-k^2\Big)\\
&=\sum_{j\ge1}\frac{(-1)^{j-1}}{j}\binom{m}{j}\left[\frac{-jm(2m-j-1)!}{(m-1)!(m-j)!}\right]\\
&=m\sum_{j\ge1}(-1)^j\binom{m}{j}\binom{2m-j-1}{m-1}=-\frac{(2m-1)!}{(m-1)!(m-1)!}.
\end{aligned}$$

Also (again by Vandermonde's formula)

$$\sum_{k=0}^{m}k\binom{m}{k}^2=\frac{(2m-1)!}{(m-1)!(m-1)!},$$

so the conjecture is proved for $\ell = 2$. With both methods just sketched one could go up to higher exponents of k. However, things become quite unwieldy.

We now present yet a third method that does enable one to deal with the general case. Recall the definition of the *falling factorials* [7, p. 47]: $x^{\underline{k}} = x(x-1)\dots(x-k+1) = x!/(x-k)!$. In order to prove the conjecture, it is equivalent to prove

$$\sum_{k=0}^{m} \frac{d}{dk}\left[k^{\underline{j}}\binom{m}{k}^2\right],$$

since ordinary powers can be expressed as linear combinations of the falling factorials and vice versa [7, pp. 262–3]. This differentiation can be explicitly described: For this, we need the extension of harmonic numbers to real or complex numbers via $H_z = \sum_{k\geq 1}\left(\frac{1}{k} - \frac{1}{k+z}\right)$, cf. [7, Ex. 6.22]. Then

$$\frac{d}{dk}k^{\underline{j}} = k^{\underline{j}}\big(H_k - H_{k-j}\big) \qquad \text{and} \qquad \frac{d}{dk}\binom{m}{k}^2 = 2\binom{m}{k}^2\big(H_{m-k} - H_k\big).$$

One must be careful and express certain quantities as an appropriate limit whenever necessary, since H_{k-j} is undefined when $k-j$ is a negative integer. Then

$$\sum_{k=0}^{m} \frac{d}{dk}\left[k^{\underline{j}}\binom{m}{k}^2\right] = \lim_{x\to 0} S_m$$

where

$$S_m := \sum_{k=0}^{m} \left(-H_k + 2H_{m-k} - H_{k-j+x}\right)\frac{k!}{(k-j+x)!}\binom{m}{k}^2.$$

Now the *Sigma* produces an (inhomogeneous) recursion of order one for S_m, namely

$$(2m+x+1-j)(2m+x+2-j)\,S_m + (m+x+1-j)S_{m+1} = \frac{(2j-3m-2x-3)(j-x)}{(m+1)(x-j)!},$$

which can be solved by iteration. The result is

$$S_m = -\frac{(2m-j+x)!}{(m-j+x)!^2}\left[H_{x-j} + \frac{1}{(x-j-1)!}\sum_{i=1}^{m}\frac{2j-2x-3i}{i}\frac{(x+i-j-1)!^2}{(x+2i-j)!}\right].$$

Taking the limit $x \to 0$, the proof of the conjecture follows by a routine analysis using formulæ such as

$$\lim_{x\to 0}\frac{H_{-j+x}}{(-j+x)!} = (j-1)!(-1)^j, \qquad \text{for } j \in \mathbb{N},$$

which belong to the repertoire of the Γ and the ψ functions, and are built-in in standard computer algebra packages.

One can also, for example from the last form, find the value $m!^2$ of S_m for $j = 2m+1$. And when performing a few computer experiments, a general pattern evolves:

$$S_{m,j} := \sum_{k=0}^{m}\frac{d}{dk}\left[k^{\underline{2m+1+j}}\binom{m}{k}^2\right] = (-1)^j\frac{(m+j)!^2}{j!} \quad \text{for } j = 0, 1, \dots .$$

The proof is easy: Because of the factor $k^{\underline{2m+1+j}}$, which is always zero for m and j in the range under consideration, we get nonzero contributions only if we differentiate it with respect to k and get rid of the factor zero. But then

$$S_{m,j} = \sum_{k=0}^{m} k!(2m+j-k)!(-1)^{k-j}\binom{m}{k}^2.$$

Now Zeilberger's algorithm produces the recurrence $S_{m,j} = (m+j)^2 S_{m-1,j}$. Since $S_{0,j} = j!(-1)^j$, the result is immediate. (The sum is basically Vandermonde's convolution.)

Another approach for proving Theorem 1 is as follows: it shows that the fact that

$$r_m(x)\log x + s_m(x) = O\big((x-1)^{2m+1}\big) \tag{26}$$

is equivalent to (25).

Note the identity (equivalent to (10))

$$\sum_{i=0}^{\ell-1}\binom{k}{i}\frac{(-1)^{\ell-1-i}}{\ell-i} = \binom{k}{\ell}\Big(H_k - H_{k-\ell}\Big),$$

and the equivalent form

$$\ell!\sum_{i=0}^{\ell-1}\binom{k}{i}\frac{(-1)^{\ell-1-i}}{\ell-i} = \frac{d}{dk}k^{\underline{\ell}}.$$

Now consider $x^k\log(x)$ and differentiate it ℓ times (D now stands for d/dx):

$$\sum_{i=0}^{\ell}\binom{\ell}{i}\{D^i x^k\}\{D^{\ell-i}\log(x)\} = \sum_{i=0}^{\ell-1}\binom{\ell}{i}k^{\underline{i}}x^{k-i}(-1)^{-1-i}(\ell-1-i)!x^{-\ell+j} + k^{\underline{\ell}}x^{k-\ell}\log(x);$$

and

$$\begin{aligned}\sum_{i=0}^{\ell}\binom{\ell}{i}\{D^i x^k\}\{D^{\ell-i}\log(x)\}\Big|_{x=1} &= \sum_{i=0}^{\ell-1}\binom{\ell}{i}k^{\underline{i}}(-1)^{-1-i}(\ell-1-i)!\\ &= \ell!\sum_{i=0}^{\ell-1}\binom{k}{i}\frac{(-1)^{\ell-1-i}}{\ell-i} = \frac{d}{dk}k^{\underline{\ell}}.\end{aligned}$$

So we have by linearity for any polynomial $\sum_k a_k x^k$

$$D^\ell\Big(\log(x)\cdot\sum_k a_k x^k\Big)\Big|_{x=1} = \sum_k a_k\frac{d}{dk}k^{\underline{\ell}}.$$

Alternatively, this formula can be proved by induction on ℓ.

Now we want to apply this to

$$r_m(x)\log(x) + s_m(x),$$

where the explicit forms of $r_m(x)$ and $s_m(x)$ are given in [24, Theorem 1]:

$$\begin{aligned}D^\ell\Big(r_m(x)\log(x) + s_m(x)\Big)\Big|_{x=1} &= \sum_{k=0}^{m}\binom{m}{k}^2\frac{d}{dk}k^{\underline{\ell}} + \sum_{k=0}^{m}k^{\underline{\ell}}\frac{d}{dk}\binom{m}{k}^2\\ &= \sum_{k=0}^{m}\frac{d}{dk}\Big[k^{\underline{\ell}}\binom{m}{k}^2\Big].\end{aligned}$$

The last step was just the product rule for differentiation. However, eq. (26) implies that

$$D^\ell\Big(r_m(x)\log(x)+s_m(x)\Big)\Big|_{x=1}=\sum_{k=0}^m\frac{d}{dk}\left[k^{\underline{\ell}}\binom{m}{k}^2\right]=0.$$

for $0\le\ell\le 2m$.

This argument can be shortened by using the operator $\delta=x\frac{d}{dx}$. We will prove the equivalent identity

$$\delta^\ell\Big(r_m(x)\log(x)+s_m(x)\Big)\Big|_{x=1}=0$$

for $0\le\ell\le 2m$. As can easily be checked, the operator δ also satisfies a Leibniz relation

$$\delta^n(fg)=\sum_{k=0}^n\binom{n}{k}(\delta^k f)(\delta^{n-k}g).$$

Also note that $\delta^\ell(x^k)\big|_{x=1}=k^\ell$, $\delta^\ell(x^k\log(x))\big|_{x=1}=\ell k^{\ell-1}=\frac{d}{dk}k^\ell$, $\delta^\ell(x^k\log^2(x))\big|_{x=1}=\ell(\ell-1)k^{\ell-2}=\frac{d^2}{dk^2}k^\ell$, etc. Now apply δ^ℓ to $r_m(x)\log(x)+s_m(x)$:

$$\delta^\ell\Big(r_m(x)\log(x)+s_m(x)\Big)\Big|_{x=1}=\sum_{k=0}^m\binom{m}{k}^2\frac{d}{dk}k^\ell+\sum_{k=0}^m k^\ell\frac{d}{dk}\binom{m}{k}^2=\sum_{k=0}^m\frac{d}{dk}\left[k^\ell\binom{m}{k}^2\right]=0$$

for $0\le\ell\le 2m$.

So differentiations (with the δ operator), evaluated at $x=1$, translate in an immediate way into differentiations of powers of k with respect to k. If we apply this to [24, Theorem 2], then we get, using the Leibniz rule with exponent 2:

$$\begin{aligned}\delta^\ell\Big(r_m(x)\log^2(x)+s_m(x)\log(x)+t_m(x)\Big)\Big|_{x=1}&=\sum_{k=0}^m(-1)^k\binom{m}{k}^3\frac{d^2}{dk^2}k^\ell\\&+2\sum_{k=0}^m(-1)^k\binom{m}{k}^3\frac{d}{dk}k^\ell+\sum_{k=0}^m(-1)^k\left[\frac{d^2}{dk^2}\binom{m}{k}^3+\pi^2\binom{m}{k}^3\right]\\&=\sum_{k=0}^m(-1)^k\Big(\frac{d^2}{dk^2}+\pi^2\Big)\left[k^\ell\binom{m}{k}^3\right]=0\end{aligned}$$

for $\ell=0,\dots,3m+1$.

It is not difficult to compute the first value (i.e., for $\ell=3m+2$) that is different from zero. Instead of k^{3m+2} we take $k^{\underline{m+1}}k^{\underline{m+1}}k^{\underline{m}}=k^{3m+2}+O(k^{3m+1})$. Now $k^{\underline{m+1}}$ is always zero, so we can only get nonzero contributions if we use the two differentiations to get rid of the factors zero. So

$$\begin{aligned}\sum_{k=0}^m(-1)^k\Big(\frac{d^2}{dk^2}+\pi^2\Big)\left[k^{3m+2}\binom{m}{k}^3\right]&=\sum_{k=0}^m(-1)^k\Big(\frac{d^2}{dk^2}+\pi^2\Big)\left[k^{\underline{m+1}}k^{\underline{m+1}}k^{\underline{m}}\binom{m}{k}^3\right]\\&=2\sum_{k=0}^m(-1)^k\big(k^{\underline{m}}\big)^3\binom{m}{k}^3=2(-1)^m m!^3,\end{aligned}$$

as only the term with $k=m$ survives.

6. A conjecture

Consider the general approximation problem

$$r_{m,n;n}(x)\big(\log x\big)^n + r_{m,n;n-1}(x)\big(\log x\big)^{n-1} + \cdots + r_{m,n;0}(x) = O\big((x-1)^{(n+1)(m+1)-1}\big),$$

where we were forced to adopt a more general notation than (1). In this section we state a conjecture about the general form of the polynomials $r_{m,n;i}(x)$.

Computer experiments lead us to the following conjecture

$$\sum_{k=0}^{m}(-1)^{(n+1)k}p_n(D)\left[k^{\ell}\binom{m}{k}^{n+1}\right]=0$$

or, equivalently in terms of falling factorials,

$$\sum_{k=0}^{m}(-1)^{(n+1)k}p_n(D)\left[k^{\underline{\ell}}\binom{m}{k}^{n+1}\right]=0 \qquad (27)$$

for $\ell = 0,\dots,n$ (initial conditions) but also $\ell = n+1,\dots,(n+1)m+1$ (implied identities). Here, $p_n(D)$ are polynomials in the differentiation operator $D = d/dk$. The first few are $p_1(D) = D$, $p_2(D) = D^2+\pi^2$ (cf. eq. (14)), $p_3(D) = D(D^2+4\pi^2)$ (cf. eq. (20)), and $p_4(D) = (D^2+\pi^2)(D^2+9\pi^2)$ (cf. eq. (24)). The general formula is (with i the complex unit)

$$p_n(D) = \prod_{k=1}^{n}\Big(D-(2k-n-1)\pi \mathrm{i}\Big).$$

The coefficient polynomials $r_{m,n;i}(x)$ can be reconstructed from (27) as follows. Computations along the lines of the previous section produce

$$D^{\ell}\big(x^k \log^i x\big)\Big|_{x=1} = \frac{d^i}{dk^i}k^{\underline{\ell}}.$$

Now $p_n(D)\big[k^{\underline{\ell}}\binom{m}{k}^{n+1}\big]$ is a linear combination of terms like $\frac{d^i}{dk^i}k^{\underline{\ell}}$; translate that formally into $x^k\log^i x$. To wit, if we set

$$p_n(D) = \sum_{j=0}^{n}\alpha_{n,j}D^j,$$

then

$$\begin{aligned}
&\sum_{k=0}^{m}(-1)^{(n+1)k}p_n(D)\left[k^{\underline{\ell}}\binom{m}{k}^{n+1}\right]\\
&=\sum_{k=0}^{m}(-1)^{(n+1)k}\sum_{j=0}^{n}\alpha_{n,j}D^j\left[k^{\underline{\ell}}\binom{m}{k}^{n+1}\right]\\
&=\sum_{k=0}^{m}(-1)^{(n+1)k}\sum_{j=0}^{n}\alpha_{n,j}\sum_{i=0}^{j}\binom{j}{i}\{D^i k^{\underline{\ell}}\}\Big\{D^{j-i}\binom{m}{k}^{n+1}\Big\}.
\end{aligned}$$

Using the translation rule described above, this becomes

$$\sum_{k=0}^{m}(-1)^{(n+1)k}\sum_{j=0}^{n}\alpha_{n,j}\sum_{i=0}^{j}\binom{j}{i}\{x^k\log^i x\}\Big\{D^{j-i}\binom{m}{k}^{n+1}\Big\}.$$

By collecting terms in $\log x$, we therefore conjecture that

$$r_{m,n;i}(x) = \sum_{k=0}^{m} (-1)^{(n+1)k} x^k \sum_{j=i}^{n} \alpha_{n,j} \binom{j}{i} \Big\{ D^{j-i} \binom{m}{k}^{n+1} \Big\}.$$

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