



Harmonic number identities and Hermite–Padé approximations to the logarithm function

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Abstract

By decomposing rational functions into partial fractions, we will establish several striking harmonic number identities including the hardest challenges discovered recently by Driver et al. [Padé approximations to the logarithm II: identities, recurrences and symbolic computation, Ramanujan J., 2003, to appear]. As application, we construct explicitly the generalized Hermite–Padé approximants to the logarithm and therefore resolve completely this open problem in the general case.

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0. Introduction

The generalized harmonic numbers are defined to be partial sums of the Riemann–Zeta series:

$$H_0^{(m)} = 0 \quad \text{and} \quad H_n^{(m)} = \sum_{k=1}^n \frac{1}{k^m} \quad \text{for} \quad m, n = 1, 2, \dots \quad (0.1)$$

When $m = 1$, they reduce to the classical ones, shortened as $H_n = H_n^{(1)}$.

If the shifted factorial is defined by

$$(c)_0 \equiv 1 \quad \text{and} \quad (c)_n = c(c+1) \cdots (c+n-1) \quad \text{for} \quad n = 1, 2, \dots$$

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then we can establish, by means of the standard partial-fraction decompositions, the following algebraic identities:

$$\frac{n!}{(x)_{n+1}} = \sum_{k=0}^n \binom{n}{k} \frac{(-1)^k}{x+k}, \tag{0.2}$$

$$\frac{(n!)^2}{(x)_{n+1}^2} = \sum_{k=0}^n \binom{n}{k}^2 \left\{ \frac{1}{(x+k)^2} + \frac{2}{x+k} (H_k - H_{n-k}) \right\}, \tag{0.3}$$

$$\frac{(n!)^3}{(x)_{n+1}^3} = \sum_{k=0}^n (-1)^k \binom{n}{k}^3 \left\{ \frac{1}{(x+k)^3} + \frac{3}{(x+k)^2} (H_k - H_{n-k}) \right. \tag{0.4a}$$

$$\left. + \frac{3}{2(x+k)} [3(H_k - H_{n-k})^2 + (H_k^{(2)} + H_{n-k}^{(2)})] \right\}. \tag{0.4b}$$

Multiplying both sides of (0.4a)–(0.4b) by x and then letting $x \rightarrow \infty$, we recover one of the hardest challenge identities:

$$\sum_{k=0}^n (-1)^k \binom{n}{k}^3 \left\{ 3(H_k - H_{n-k})^2 + (H_k^{(2)} + H_{n-k}^{(2)}) \right\} = 0 \tag{0.5}$$

conjectured by Weideman [14, Eq. (20)] and proved by Schneider [6, Eq. (16)] (cf. [7, Eq. (12)] also) through computer algebra package *Sigma*.

This has best exemplified the power of partial fraction method. In general we will derive the decompositions of higher powers of such rational functions into partial fractions which involve the complete Bell polynomials (or cyclic indicators of symmetric groups) on the generalized harmonic numbers. This will be accomplished in the first section. Then Section 2 will be devoted to the partial fraction expansions of functions weighted with numerator monomials. As application, the generalized Hermite–Padé approximants to the logarithm will be constructed explicitly in the last section, which resolves this open problem completely.

1. Partial fraction decompositions

Based on nonnegative integer vectors, we introduce the coordinate sums, factorial product and the associated partition as follows:

$$\begin{aligned} \tilde{m} &= (m_1, m_2, \dots, m_\ell), \\ \tilde{m}! &= m_1! m_2! \cdots m_\ell!, \\ |\tilde{m}| &= m_1 + m_2 + \cdots + m_\ell, \\ \|\tilde{m}\| &= m_1 + 2m_2 + \cdots + \ell m_\ell. \end{aligned}$$

1.1. Partial Bell polynomials and Faà di Bruno formula

For the ℓ -partition represented by multiset $\{1^{m_1}, 2^{m_2}, \dots, \ell^{m_\ell}\}$ and determined by ℓ -tuples of nonnegative integers $\tilde{m} = (m_1, m_2, \dots, m_\ell)$, let $|\tilde{m}| = \sum_{i=1}^\ell m_i$ and $\|\tilde{m}\| = \sum_{i=1}^\ell i m_i$ stand for the length and the weight of the partition, respectively. Then partial Bell polynomials associated

with f -function are defined by

$$B_{m,\ell}(f) = \sum_{\substack{\|\vec{m}\|=\ell \\ \vec{m}=m}} \frac{\ell!}{\vec{m}!} \prod_{i=1}^{\ell} \left\{ \frac{f^{(i)}(x)}{i!} \right\}^{m_i}, \quad m, \ell = 1, 2, \dots, \tag{1.1}$$

where as usual we denote the n th derivative of function $F(x)$ by

$$F^{(n)}(x) = \mathcal{D}_x^n F(x) \quad \text{with} \quad \mathcal{D}_x = \frac{d}{dx}.$$

For composite functions, their derivatives of higher order are provided by the following well-known result:

Lemma 1 (Faà di Bruno formula [4, p. 139]). *For two ℓ -times differentiable functions $f(x)$ and $\phi(x)$, let F be the composite function*

$$F(x) := \phi \circ f(x) = \phi[f(x)].$$

Then F is also ℓ -times differentiable function with

$$F^{(\ell)}(x) = \sum_{m=0}^{\ell} \phi^{(m)}[f(x)] B_{m,\ell}(f). \tag{1.2}$$

1.2. Partial fraction decomposition

In order to proceed smoothly on the investigation of partial fraction expansion, we fix a rational function

$$h(x) = \frac{n! \times (x+k)}{(x)_{n+1}} = \frac{n!}{(x)_k (1+x+k)_{n-k}} \tag{1.3}$$

and define further a function related to harmonic numbers

$$\mathcal{H}_\ell(x) = \sum_{\substack{i=0 \\ i \neq k}}^n \frac{1}{(x+i)^\ell}, \tag{1.4a}$$

$$\mathcal{H}_\ell(-k) = H_{n-k}^{(\ell)} + (-1)^\ell H_k^{(\ell)}. \tag{1.4b}$$

Now we are ready to state our main result as the following:

Theorem 2 (Partial fraction decomposition). *Let λ and n be two natural numbers. Then there holds the algebraic identity:*

$$\frac{(n!)^\lambda}{(x)_{n+1}^\lambda} = \sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \sum_{\ell=0}^{\lambda-1} \frac{\omega_\ell(\lambda, -k)}{\ell! \times (x+k)^{\lambda-\ell}}, \tag{1.5}$$

where the ω -coefficients are determined by the logarithmic derivative:

$$\omega_\ell(\lambda, x) := \frac{\mathcal{D}_x^\ell h^\lambda(x)}{h^\lambda(x)} = (-1)^\ell \ell! \sum_{\|\vec{m}\|=\ell} \frac{\lambda^{|\vec{m}|}}{\vec{m}!} \prod_{i=1}^{\ell} \frac{\mathcal{H}_i^{m_i}(x)}{i^{m_i}}, \tag{1.6a}$$

$$\omega_\ell(\lambda, -k) = \ell! \sum_{\|\tilde{m}\|=\ell} \frac{\lambda^{|\tilde{m}|}}{\tilde{m}!} \prod_{i=1}^{\ell} \frac{\{H_k^{(i)} + (-1)^i H_{n-k}^{(i)}\}^{m_i}}{i^{m_i}}. \tag{1.6b}$$

Proof. By means of partial fraction decomposition, we can formally write

$$\frac{(n!)^\lambda}{(x)_{n+1}^\lambda} = \sum_{k=0}^n \sum_{\ell=0}^{\lambda-1} \frac{C(k, \ell)}{(x+k)^{\lambda-\ell}},$$

where the coefficients $C(k, \ell)$ are to be determined. Noting that

$$h^\lambda(-k) = (-1)^{k\lambda} \binom{n}{k}^\lambda$$

we need only to check that for $0 \leq \ell < \lambda$ there holds:

$$C(k, \ell) = h^\lambda(-k) \times \frac{\omega_\ell(\lambda, -k)}{\ell!} \quad \text{with} \quad \omega_\ell(\lambda, -k) = \left. \frac{\mathcal{D}_x^\ell h^\lambda(x)}{h^\lambda(x)} \right|_{x=-k}. \tag{1.7}$$

For $\ell = 0$, we have obviously $\omega_0(\lambda, x) \equiv 1$ and that

$$C(k, 0) = \lim_{x \rightarrow -k} h^\lambda(x) = h^\lambda(-k) \times \omega_0(\lambda, -k).$$

Next for $\ell = 1$, we can compute through L'Hospital's rule that

$$\begin{aligned} C(k, 1) &= \lim_{x \rightarrow -k} (x+k)^{\lambda-1} \left\{ \frac{(n!)^\lambda}{(x)_{n+1}^\lambda} - \frac{C(k, 0)}{(x+k)^\lambda} \right\} \\ &= \lim_{x \rightarrow -k} \frac{h^\lambda(x) - C(k, 0)}{x+k} = \lim_{x \rightarrow -k} \mathcal{D}_x h^\lambda(x) \\ &= \lim_{x \rightarrow -k} h^\lambda(x) \frac{\mathcal{D}_x h^\lambda(x)}{h^\lambda(x)} = h^\lambda(-k) \times \omega_1(\lambda, -k). \end{aligned}$$

Suppose that $C(k, \ell) = h^\lambda(-k) \times \omega_\ell(\lambda, -k)$ is true for $\ell = 0, 1, \dots, m-1$ with $m < \lambda$. Then we have to verify it also for $\ell = m$. Applying again the L'Hospital rule for m -times, we can determine the coefficient

$$\begin{aligned} C(k, m) &= \lim_{x \rightarrow -k} (x+k)^{\lambda-m} \left\{ \frac{(n!)^\lambda}{(x)_{n+1}^\lambda} - \sum_{\ell=0}^{m-1} \frac{C(k, \ell)}{(x+k)^{\lambda-\ell}} \right\} \\ &= \lim_{x \rightarrow -k} \frac{1}{(x+k)^m} \left\{ h^\lambda(x) - \sum_{\ell=0}^{m-1} C(k, \ell) \times (x+k)^\ell \right\} \\ &= \lim_{x \rightarrow -k} h^\lambda(x) \frac{\mathcal{D}_x^m h^\lambda(x)}{m! h^\lambda(x)} = h^\lambda(-k) \times \frac{\omega_m(\lambda, -k)}{m!}. \end{aligned}$$

Based on the induction principle, we have confirmed that the coefficients in partial fraction decomposition are determined by (1.7).

To complete the proof of the theorem, it remains to show that these coefficients can be calculated concretely through the RHS of Eq. (1.6a) and so (1.6b), the partial Bell polynomials.

In Lemma 1, specifying the composite function with

$$\phi(y) = e^{\lambda y} \quad \text{and} \quad f(x) = \ln h(x)$$

we can compute without difficulty their derivatives

$$\frac{D_y^m \phi(y)}{\phi(y)} = \lambda^m \quad \text{and} \quad D_x^\kappa f(x) = (-1)^\kappa (\kappa - 1)! \mathcal{H}_\kappa(x)$$

as well as the partial Bell polynomials

$$B_{m,\ell}(f) = (-1)^\ell \sum_{\substack{\|\tilde{m}\|=\ell \\ |\tilde{m}|=m}} \frac{\ell!}{\tilde{m}!} \prod_{i=1}^\ell \frac{\mathcal{H}_i^{m_i}(x)}{i^{m_i}}$$

which leads us immediately to (1.6a):

$$\omega_\ell(\lambda, x) = \frac{D_x^\ell h^\lambda(x)}{h^\lambda(x)} = (-1)^\ell \ell! \sum_{\|\tilde{m}\|=\ell} \frac{\lambda^{|\tilde{m}|}}{\tilde{m}!} \prod_{i=1}^\ell \frac{\mathcal{H}_i^{m_i}(x)}{i^{m_i}}.$$

This completes the proof of Theorem 2. \square

1.3. Harmonic number identities

In Theorem 2, multiplying both sides by x and then letting $x \rightarrow \infty$, we find the following general identity on harmonic numbers.

Corollary 3 (Combinatorial identity on harmonic numbers). *For two natural numbers λ and n , there holds*

$$0 \equiv \sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \omega_{\lambda-1}(\lambda, -k). \tag{1.8}$$

When $\lambda = 3$, it reduces to a conjectured formula due to Weideman [14, Eq. (20)]

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

which has been confirmed recently via symbolic calculus and computer algebra by Driver et al. [6], who declared it as one of the hardest challenges to prove.

Noticing from (1.6b) that

$$\omega_\ell(\lambda, k - n) = (-1)^\ell \omega_\ell(\lambda, -k) \tag{1.9}$$

we have similarly the following limiting relation:

$$\begin{aligned} & \sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \frac{\omega_{\lambda-2}(\lambda, -k)}{(\lambda - 2)!} \\ &= \lim_{x \rightarrow \infty} x^2 \left\{ \frac{(n!)^\lambda}{(x)_{n+1}^\lambda} - \sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \frac{\omega_{\lambda-1}(\lambda, -k)}{(\lambda - 1)! (x + k)} \right\} \end{aligned}$$

$$\begin{aligned}
 &= \lim_{x \rightarrow \infty} x^2 \left\{ \sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \frac{-\omega_{\lambda-1}(\lambda, -k)}{(\lambda-1)! (x+k)} \right\} \\
 &= \lim_{x \rightarrow \infty} \sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \frac{\omega_{\lambda-1}(\lambda, -k)}{(\lambda-1)!} \\
 &\quad \times \frac{x^2}{2} \left\{ \frac{-1}{x+k} + \frac{(-1)^{\lambda(n+1)}}{x+n-k} \right\},
 \end{aligned}$$

where the involution $k \rightarrow n - k$ has been performed in the last passage.

Combining with two further relations:

$$\begin{aligned}
 &\sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \omega_{\lambda-2}(\lambda, -k) = 0, \quad \lambda(n+1)\text{-odd}, \\
 &\lim_{x \rightarrow \infty} x^2 \left\{ \frac{-1}{x+k} + \frac{(-1)^{\lambda(n+1)}}{x+n-k} \right\} = 2k - n, \quad \lambda(n+1)\text{-even},
 \end{aligned}$$

we derive from Theorem 2 the following curious identities:

Proposition 4 (Two curious identities).

$$\lim_{x \rightarrow \infty} x^3 \sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \frac{\omega_{\lambda-1}(\lambda, -k)}{(x+k)(x+n-k)} \equiv 0, \quad \lambda\text{-odd}, \tag{1.10a}$$

$$\sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \left\{ \begin{aligned} &(n-2k) \omega_{\lambda-1}(\lambda, -k) \\ &+ 2(\lambda-1) \omega_{\lambda-2}(\lambda, -k) \end{aligned} \right\} \equiv 0, \quad \lambda\text{-even}. \tag{1.10b}$$

Even for $\lambda = 1$, the limiting relation (1.10a) yields a non-trivial result:

$$0 = \lim_{x \rightarrow \infty} \sum_{k=0}^n (-1)^k \binom{n}{k} \frac{x^3}{(x+k)(x+n-k)}, \tag{1.11}$$

which can be verified by means of finite differences

$$\sum_{k=0}^n \binom{n}{k} \frac{(-1)^k}{x+k} = \frac{n!}{(x)_{n+1}} \tag{1.12}$$

in view of the Newton–Gregory formula and induction principle.

When $\lambda = 2$, equality (1.10b) reads explicitly as

$$\binom{2n}{n} = \sum_{k=0}^n (2k-n) \binom{n}{k}^2 \{H_k - H_{n-k}\}. \tag{1.13}$$

For $\lambda = 3$, the limiting relation (1.10a) yields another formula:

$$0 = \lim_{x \rightarrow \infty} x^3 \sum_{k=0}^n (-1)^k \binom{n}{k}^3 \frac{3(H_k - H_{n-k})^2 + (H_k^{(2)} + H_{n-k}^{(2)})}{(x+k)(x+n-k)}. \tag{1.14}$$

The present author is unable to show it directly.

When $\lambda = 4$, equality (1.10b) reads explicitly as

$$0 = \sum_{k=0}^n \binom{n}{k}^4 \left\{ 12(H_k - H_{n-k})^2 + 3(H_k^{(2)} + H_{n-k}^{(2)}) \right. \tag{1.15a}$$

$$\left. + (n-2k) \left[8(H_k - H_{n-k})^3 + (H_k^{(3)} - H_{n-k}^{(3)}) \right] \right\} \tag{1.15b}$$

which is equivalent, under involution $k \rightarrow n - k$, to the identity discovered by Driver et al. [6, p. 9] and [7, Eq. (21)] with the symbolic summation package *Sigma*.

1.4. Partial Bell polynomials

According to (1.6a), we display the first few examples as follows:

$$+ \omega_0(\lambda, x) \equiv 1, \tag{1.16}$$

$$- \omega_1(\lambda, x) = \lambda \mathcal{H}_1, \tag{1.17}$$

$$+ \omega_2(\lambda, x) = \lambda^2 \mathcal{H}_1^2 + \lambda \mathcal{H}_2, \tag{1.18}$$

$$- \omega_3(\lambda, x) = \lambda^3 \mathcal{H}_1^3 + 3\lambda^2 \mathcal{H}_1^2 \mathcal{H}_2 + 2\lambda \mathcal{H}_3, \tag{1.19}$$

$$+ \omega_4(\lambda, x) = \lambda^4 \mathcal{H}_1^4 + 6\lambda^3 \mathcal{H}_1^2 \mathcal{H}_2 + 8\lambda^2 \mathcal{H}_1 \mathcal{H}_3 + 3\lambda^2 \mathcal{H}_2^2 + 6\lambda \mathcal{H}_4, \tag{1.20}$$

$$- \omega_5(\lambda, x) = \lambda^5 \mathcal{H}_1^5 + 10\lambda^4 \mathcal{H}_1^3 \mathcal{H}_2 + 20\lambda^3 \mathcal{H}_1^2 \mathcal{H}_3 + 15\lambda^3 \mathcal{H}_1 \mathcal{H}_2^2 \tag{1.21a}$$

$$+ 30\lambda^2 \mathcal{H}_1 \mathcal{H}_4 + 20\lambda^2 \mathcal{H}_2 \mathcal{H}_3 + 24\lambda \mathcal{H}_5. \tag{1.21b}$$

Under replacement (1.4b), their particular values (1.6b) can be produced as follows:

$$\omega_0(\lambda, -k) \equiv 1, \tag{1.22}$$

$$\omega_1(\lambda, -k) = \lambda \{ H_k - H_{n-k} \}, \tag{1.23}$$

$$\omega_2(\lambda, -k) = \lambda^2 \{ H_k - H_{n-k} \}^2 + \lambda \{ H_k^{(2)} + H_{n-k}^{(2)} \}, \tag{1.24}$$

$$\omega_3(\lambda, -k) = \lambda^3 \{ H_k - H_{n-k} \}^3 + 2\lambda \{ H_k^{(3)} - H_{n-k}^{(3)} \} \tag{1.25a}$$

$$+ 3\lambda^2 \{ H_k - H_{n-k} \} \times \{ H_k^{(2)} + H_{n-k}^{(2)} \}, \tag{1.25b}$$

$$\omega_4(\lambda, -k) = \lambda^4 \{ H_k - H_{n-k} \}^4 + 6\lambda \{ H_k^{(4)} + H_{n-k}^{(4)} \} \tag{1.26a}$$

$$+ 8\lambda^2 \{ H_k - H_{n-k} \} \times \{ H_k^{(3)} - H_{n-k}^{(3)} \} \tag{1.26b}$$

$$+ 6\lambda^3 \{ H_k - H_{n-k} \}^2 \times \{ H_k^{(2)} + H_{n-k}^{(2)} \} \tag{1.26c}$$

$$+ 3\lambda^2 \{ H_k^{(2)} + H_{n-k}^{(2)} \}^2, \tag{1.26d}$$

$$\omega_5(\lambda, -k) = \lambda^5 \{ H_k - H_{n-k} \}^5 + 24\lambda \{ H_k^{(5)} - H_{n-k}^{(5)} \} \tag{1.27a}$$

$$+ 10\lambda^4 \{ H_k - H_{n-k} \}^3 \times \{ H_k^{(2)} + H_{n-k}^{(2)} \} \tag{1.27b}$$

$$+ 20\lambda^3 \{H_k - H_{n-k}\}^2 \times \{H_k^{(3)} - H_{n-k}^{(3)}\} \tag{1.27c}$$

$$+ 15\lambda^3 \{H_k - H_{n-k}\} \times \{H_k^{(2)} + H_{n-k}^{(2)}\}^2 \tag{1.27d}$$

$$+ 30\lambda^2 \{H_k - H_{n-k}\} \times \{H_k^{(4)} + H_{n-k}^{(4)}\} \tag{1.27e}$$

$$+ 20\lambda^2 \{H_k^{(2)} + H_{n-k}^{(2)}\} \times \{H_k^{(3)} - H_{n-k}^{(3)}\}. \tag{1.27f}$$

1.5. Further expansion and identity

In view of Theorem 2, Corollary 3 and Proposition 4, we can display the fifth partial fraction expansion

$$\frac{(n!)^5}{(x)_{n+1}^5} = \sum_{k=0}^n (-1)^k \binom{n}{k}^5 \left\{ \frac{1}{(x+k)^5} + \frac{5}{(x+k)^4} (H_k - H_{n-k}) \right. \tag{1.28a}$$

$$\left. + \frac{5}{2(x+k)^3} \left[5(H_k - H_{n-k})^2 + (H_k^{(2)} + H_{n-k}^{(2)}) \right] \right. \tag{1.28b}$$

$$\left. + \frac{5}{6(x+k)^2} \left[\begin{matrix} 25(H_k - H_{n-k})^3 + 2(H_k^{(3)} - H_{n-k}^{(3)}) \\ + 15(H_k - H_{n-k})(H_k^{(2)} + H_{n-k}^{(2)}) \end{matrix} \right] \right. \tag{1.28c}$$

$$\left. + \frac{5}{24(x+k)} \left[\begin{matrix} 150(H_k - H_{n-k})^2(H_k^{(2)} + H_{n-k}^{(2)}) + 40(H_k - H_{n-k})(H_k^{(3)} - H_{n-k}^{(3)}) \\ + 125(H_k - H_{n-k})^4 + 15(H_k^{(2)} + H_{n-k}^{(2)})^2 + 6(H_k^{(4)} + H_{n-k}^{(4)}) \end{matrix} \right] \right\} \tag{1.28d}$$

and the corresponding harmonic number identity

$$0 = \sum_{k=0}^n (-1)^k \binom{n}{k}^5 \left\{ \begin{matrix} 150(H_k - H_{n-k})^2(H_k^{(2)} + H_{n-k}^{(2)}) + 40(H_k - H_{n-k})(H_k^{(3)} - H_{n-k}^{(3)}) \\ + 125(H_k - H_{n-k})^4 + 15(H_k^{(2)} + H_{n-k}^{(2)})^2 + 6(H_k^{(4)} + H_{n-k}^{(4)}) \end{matrix} \right\} \tag{1.29}$$

as well as the limiting relation

$$0 = \lim_{x \rightarrow \infty} \sum_{k=0}^n (-1)^k \binom{n}{k}^5 \frac{x^3}{(x+k)(x+n-k)} \tag{1.30a}$$

$$\times \left\{ \begin{matrix} 150(H_k - H_{n-k})^2(H_k^{(2)} + H_{n-k}^{(2)}) + 40(H_k - H_{n-k})(H_k^{(3)} - H_{n-k}^{(3)}) \\ + 125(H_k - H_{n-k})^4 + 15(H_k^{(2)} + H_{n-k}^{(2)})^2 + 6(H_k^{(4)} + H_{n-k}^{(4)}) \end{matrix} \right\}. \tag{1.30b}$$

2. Decompositions with numerator monomials

Similar to the proof of Theorem 2, we can slightly extend it to the following form.

Theorem 5 (Partial fraction decomposition). *Let λ , θ and n be three natural numbers with $0 \leq \theta < \lambda(n + 1)$. Then there holds the algebraic identity:*

$$\frac{(n!)^\lambda x^\theta}{(x)_{n+1}^\lambda} = \sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \sum_{\ell=0}^{\lambda-1} \frac{\Omega_\ell(\lambda, \theta, -k)}{\ell! (x+k)^{\lambda-\ell}},$$

where the Ω -coefficients are determined by

$$\Omega_\ell(\lambda, \theta, x) := x^{\theta-\ell} \sum_{\|\tilde{m}\|=\ell} (-1)^{\ell+|\tilde{m}|} \frac{\ell!}{\tilde{m}!} \prod_{i=1}^\ell \frac{\{\theta - \lambda x^i \mathcal{H}_i(x)\}^{m_i}}{i^{m_i}}, \tag{2.1a}$$

$$\Omega_\ell(\lambda, \theta, -k) = k^{\theta-\ell} \sum_{\|\tilde{m}\|=\ell} (-1)^{\theta+|\tilde{m}|} \frac{\ell!}{\tilde{m}!} \prod_{i=1}^\ell \frac{\{\theta - \lambda k^i [H_k^{(i)} + (-1)^i H_{n-k}^{(i)}]\}^{m_i}}{i^{m_i}}. \tag{2.1b}$$

When $\theta = 0$, we remark that this theorem reduces to Theorem 2.

Proof of Theorem 5. Following the same process for Theorem 2, we can show that the coefficients are provided by following derivatives:

$$\Omega_\ell(\lambda, \theta, -k) := \frac{\mathcal{D}_x^\ell \{h^\lambda(x)x^\theta\}}{h^\lambda(x)} \Big|_{x=-k}. \tag{2.2}$$

Specifying the composite function in Lemma 1 with

$$\phi(y) = e^{\lambda y} \quad \text{and} \quad f(x) = \ln \left\{ x^{\theta/\lambda} h(x) \right\}.$$

we can write down their derivatives as follows

$$\frac{D_y^m \phi(y)}{\phi(y)} = \lambda^m \quad \text{and} \quad D_x^\kappa f(x) = (-1)^{\kappa-1} \frac{(\kappa-1)!}{\lambda x^\kappa} \left\{ \theta - \lambda x^\kappa \mathcal{H}_\kappa(x) \right\},$$

which allow us to determine also the partial Bell polynomials

$$B_{m,\ell}(f) = \frac{(-1)^{m+\ell}}{\lambda^m x^\ell} \sum_{\substack{\|\tilde{m}\|=\ell \\ |\tilde{m}|=m}} \frac{\ell!}{\tilde{m}!} \prod_{i=1}^\ell \frac{\{\theta - \lambda x^i \mathcal{H}_i(x)\}^{m_i}}{i^{m_i}}.$$

Then the corresponding coefficients are given as

$$\frac{\mathcal{D}_x^\ell \{h^\lambda(x)x^\theta\}}{h^\lambda(x)} = x^{\theta-\ell} \sum_{\|\tilde{m}\|=\ell} (-1)^{\ell+|\tilde{m}|} \frac{\ell!}{\tilde{m}!} \prod_{i=1}^\ell \frac{\{\theta - \lambda x^i \mathcal{H}_i(x)\}^{m_i}}{i^{m_i}}.$$

The combination of (2.2) and the last expression results directly in (2.1a).

This completes the proof of Theorem 5. \square

Applying the Leibniz rule on derivatives of two-function-product, we can establish the following relation on connection coefficients.

Proposition 6 (Relation between Bell polynomials).

$$\Omega_\ell(\lambda, \theta, x) := \sum_{i=0}^\ell x^{\theta-i} \binom{\theta}{i} \binom{\ell}{i} i! \omega_{\ell-i}(\lambda, x). \tag{2.3}$$

Multiplying both sides of the partial fraction expansion in Theorem 5 by x and then letting $x \rightarrow \infty$, we establish the following identity on harmonic numbers:

Corollary 7 (Harmonic number identity). Let λ, n and θ be three natural numbers with $1 + \theta < \lambda(n + 1)$. Then there holds the algebraic identity:

$$\sum_{k=0}^n (-1)^{k\lambda} \binom{n}{k}^\lambda \Omega_{\lambda-1}(\lambda, \theta, -k) = \begin{cases} 0, & 0 \leq \theta < \lambda(n + 1) - 1, \\ (n!)^\lambda, & \theta = \lambda(n + 1) - 1. \end{cases}$$

The first few coefficients may be displayed as follows:

$$\Omega_0(\lambda, \theta, x) = x^\theta, \tag{2.4}$$

$$\Omega_1(\lambda, \theta, x) = x^{\theta-1} \{ \theta - \lambda x \mathcal{H}_1 \}, \tag{2.5}$$

$$\Omega_2(\lambda, \theta, x) = x^{\theta-2} \left\{ (\theta - \lambda x \mathcal{H}_1)^2 - (\theta - \lambda x^2 \mathcal{H}_2) \right\}, \tag{2.6}$$

$$\Omega_3(\lambda, \theta, x) = x^{\theta-3} \left\{ \begin{array}{l} (\theta - \lambda x \mathcal{H}_1)^3 + 2(\theta - \lambda x^3 \mathcal{H}_3) \\ -3(\theta - \lambda x \mathcal{H}_1)(\theta - \lambda x^2 \mathcal{H}_2) \end{array} \right\}, \tag{2.7}$$

$$\Omega_4(\lambda, \theta, x) = x^{\theta-4} \left\{ \begin{array}{l} (\theta - \lambda x \mathcal{H}_1)^4 + 3(\theta - \lambda x^2 \mathcal{H}_2)^2 - 6(\theta - \lambda x^4 \mathcal{H}_4) \\ -6(\theta - \lambda x \mathcal{H}_1)^2(\theta - \lambda x^2 \mathcal{H}_2) + 8(\theta - \lambda x \mathcal{H}_1)(\theta - \lambda x^3 \mathcal{H}_3) \end{array} \right\}, \tag{2.8}$$

$$\Omega_5(\lambda, \theta, x) = x^{\theta-5} \left\{ \begin{array}{l} (\theta - \lambda x \mathcal{H}_1)^5 + 24(\theta - \lambda x^5 \mathcal{H}_5) + 15(\theta - \lambda x \mathcal{H}_1)(\theta - \lambda x^2 \mathcal{H}_2)^2 \\ -10(\theta - \lambda x \mathcal{H}_1)^3(\theta - \lambda x^2 \mathcal{H}_2) - 30(\theta - \lambda x \mathcal{H}_1)(\theta - \lambda x^4 \mathcal{H}_4) \\ -20(\theta - \lambda x^2 \mathcal{H}_2)(\theta - \lambda x^3 \mathcal{H}_3) + 20(\theta - \lambda x \mathcal{H}_1)^2(\theta - \lambda x^3 \mathcal{H}_3) \end{array} \right\}. \tag{2.9}$$

According to Theorem 5 and Corollary 7, we can exhibit the following expansion formulae and the corresponding harmonic number identities.

Example 1 (Partial-fraction decomposition: $\theta \leq n$).

$$\frac{n! x^\theta}{(x)_{n+1}} = \sum_{k=0}^n (-1)^{k+\theta} \binom{n}{k} \frac{k^\theta}{x+k}, \tag{2.10a}$$

$$\sum_{k=0}^n (-1)^{k+\theta} \binom{n}{k} k^\theta = \begin{cases} 0, & 0 \leq \theta < n, \\ n!, & \theta = n. \end{cases} \tag{2.10b}$$

We remark that these two identities can also be verified through finite differences.

Example 2 (Partial-fraction decomposition: $\theta < 2 + 2n$).

$$\frac{(n!)^2 x^\theta}{(x)_{n+1}^2} = \sum_{k=0}^n \binom{n}{k}^2 \left\{ \frac{(-k)^\theta}{(x+k)^2} + \frac{(-k)^{\theta-1}}{x+k} \left[\theta - 2k(H_k - H_{n-k}) \right] \right\}, \tag{2.11a}$$

$$\sum_{k=0}^n k^{\theta-1} \binom{n}{k}^2 \left\{ \theta - 2k(H_k - H_{n-k}) \right\} = \begin{cases} 0, & 0 \leq \theta \leq 2n, \\ (n!)^2, & \theta = 1 + 2n. \end{cases} \tag{2.11b}$$

Among these results, the last identity has been conjectured by Weideman [14, Eq. (11)] and proved in [6, Theorem 1].

Example 3 (Partial-fraction decomposition: $\theta < 3 + 3n$).

$$\frac{(n!)^3 x^\theta}{(x)_{n+1}^3} = \sum_{k=0}^n (-1)^k \binom{n}{k}^3 \left\{ \frac{(-k)^\theta}{(x+k)^3} + \frac{(-k)^{\theta-1}}{(x+k)^2} [\theta - 3k(H_k - H_{n-k})] \right\} \tag{2.12a}$$

$$+ \frac{(-k)^{\theta-2}}{2(x+k)} \left[\{\theta - 3k(H_k - H_{n-k})\}^2 - \theta + 3k^2(H_k^{(2)} + H_{n-k}^{(2)}) \right], \tag{2.12b}$$

$$\sum_{k=0}^n (-1)^k \binom{n}{k}^3 k^{\theta-2} \left\{ \begin{matrix} [\theta - 3k(H_k - H_{n-k})]^2 \\ -\theta + 3k^2(H_k^{(2)} + H_{n-k}^{(2)}) \end{matrix} \right\} = \begin{cases} 0, & 0 \leq \theta \leq 1 + 3n, \\ 2(n!)^3 (-1)^n, & \theta = 2 + 3n. \end{cases} \tag{2.12c}$$

In particular, the cases $\theta = 0$ and 1 of the last identity have been conjectured by Weideman [14, Eq. (20)] and then verified in [6, Eqs. (16) and (17)]. An alternative approach for (2.12c) can be found in [6, p. 15].

Example 4 (Partial-fraction decomposition: $\theta < 4 + 4n$).

$$\frac{(n!)^4 x^\theta}{(x)_{n+1}^4} = \sum_{k=0}^n \binom{n}{k}^4 \left\{ \frac{(-k)^\theta}{(x+k)^4} + \frac{(-k)^{\theta-1}}{(x+k)^3} [\theta - 4k(H_k - H_{n-k})] \right\} \tag{2.13a}$$

$$+ \frac{(-k)^{\theta-2}}{2(x+k)^2} \left[\{\theta - 4k(H_k - H_{n-k})\}^2 - \{\theta - 4k^2(H_k^{(2)} + H_{n-k}^{(2)})\} \right] \tag{2.13b}$$

$$+ \frac{(-k)^{\theta-3}}{6(x+k)} \left[\begin{matrix} \{\theta - 4k(H_k - H_{n-k})\}^3 + 2\{\theta - 4k^3(H_k^{(3)} - H_{n-k}^{(3)})\} \\ -3\{\theta - 4k(H_k - H_{n-k})\} \{\theta - 4k^2(H_k^{(2)} + H_{n-k}^{(2)})\} \end{matrix} \right]. \tag{2.13c}$$

The corresponding harmonic identity reads as

$$\sum_{k=0}^n k^{\theta-3} \binom{n}{k}^4 \left[\begin{matrix} \{\theta - 4k(H_k - H_{n-k})\}^3 + 2\{\theta - 4k^3(H_k^{(3)} - H_{n-k}^{(3)})\} \\ -3\{\theta - 4k(H_k - H_{n-k})\} \{\theta - 4k^2(H_k^{(2)} + H_{n-k}^{(2)})\} \end{matrix} \right] \tag{2.14a}$$

$$= \begin{cases} 0, & 0 \leq \theta \leq 2 + 4n, \\ 6(n!)^4, & \theta = 3 + 4n. \end{cases} \tag{2.14b}$$

For $\theta = 0, 1, 2$, the corresponding results to this identity have been conjectured by Weideman [14, Eq. (21)] and subsequently confirmed by Driver et al. [6, Eq. (20)]. In particular, we recover again, with the case $\theta = 1$, identity (1.15a)–(1.15b) found originally by Driver et al. [7, Eq. (21)].

Example 5 (Partial-fraction decomposition: $\theta < 5 + 5n$).

$$\frac{(n!)^5 x^\theta}{(x)_{n+1}^5} = \sum_{k=0}^n (-1)^k \binom{n}{k}^5 \left\{ \frac{(-k)^\theta}{(x+k)^5} + \frac{(-k)^{\theta-1}}{(x+k)^4} [\theta - 5k(H_k - H_{n-k})] \right\}$$

$$+ \frac{(-k)^{\theta-2}}{2(x+k)^3} \left[\{\theta - 5k(H_k - H_{n-k})\}^2 - \{\theta - 5k^2(H_k^{(2)} + H_{n-k}^{(2)})\} \right]$$

$$+ \frac{(-k)^{\theta-3}}{6(x+k)^2} \left[\begin{matrix} \{\theta - 5k(H_k - H_{n-k})\}^3 + 2\{\theta - 5k^3(H_k^{(3)} - H_{n-k}^{(3)})\} \\ -3\{\theta - 5k(H_k - H_{n-k})\} \{\theta - 5k^2(H_k^{(2)} + H_{n-k}^{(2)})\} \end{matrix} \right]$$

$$+ \frac{(-k)^{\theta-4}}{24(x+k)} \left[\begin{array}{l} \left\{ \begin{array}{l} \{\theta-5k(H_k-H_{n-k})\}^4 - 6\{\theta-5k^4(H_k^{(4)}+H_{n-k}^{(4)})\} \\ -6\{\theta-5k(H_k-H_{n-k})\}^2 \{\theta-5k^2(H_k^{(2)}+H_{n-k}^{(2)})\} \\ +8\{\theta-5k(H_k-H_{n-k})\} \times \{\theta-5k^3(H_k^{(3)}-H_{n-k}^{(3)})\} \\ +3\{\theta-5k^2(H_k^{(2)}+H_{n-k}^{(2)})\}^2 \end{array} \right\} \end{array} \right].$$

The corresponding harmonic identity reads as

$$\sum_{k=0}^n (-1)^k \binom{n}{k}^5 k^{\theta-4} \left\{ \begin{array}{l} \{\theta-5k(H_k-H_{n-k})\}^4 - 6\{\theta-5k^4(H_k^{(4)}+H_{n-k}^{(4)})\} \\ -6\{\theta-5k(H_k-H_{n-k})\}^2 \{\theta-5k^2(H_k^{(2)}+H_{n-k}^{(2)})\} \\ +8\{\theta-5k(H_k-H_{n-k})\} \times \{\theta-5k^3(H_k^{(3)}-H_{n-k}^{(3)})\} \\ +3\{\theta-5k^2(H_k^{(2)}+H_{n-k}^{(2)})\}^2 \end{array} \right\} \tag{2.15a}$$

$$= \begin{cases} 0, & 0 \leq \theta \leq 3 + 5n, \\ 24(n!)^5 (-1)^n, & \theta = 4 + 5n. \end{cases} \tag{2.15b}$$

The cases corresponding to $\theta = 0, 1, 2, 3$ have been conjectured by Weideman [14, Eq. (22)] and claimed subsequently to be verified by Driver et al. [6, p. 11] and Weideman [15] through computer algebra package *Sigma*.

3. Hermite–Padé approximations to the logarithm based at $x = 1$

For given positive integers m and n , the problem consists of finding $m + 1$ polynomials $\{ {}_m P_\ell(x) \}_{\ell=0}^m$ of degree at most n such that

$$\sum_{\ell=0}^m {}_m P_\ell(x) (\ln x)^{m-\ell} = \mathcal{O}\left\{ (x-1)^{m+n+mn} \right\}. \tag{3.1}$$

Weideman [14] has derived the explicit formula for the quadratic approximation and characterized the cubic and quartic cases, which have been resolved subsequently in [6,7], where recurrence relations for computations have been investigated through computer algebra package *Sigma* as proposed first by Borwein [2]. Based on the Bell polynomials $\omega_\ell(\lambda, x)$ introduced in this paper, we will explicitly construct the generalized Hermite–Padé approximants to the logarithm and therefore resolve this open problem completely.

Theorem 8 (*Padé approximations to the logarithm*). For $0 \leq \ell \leq m$, define the Padé approximants by

$${}_m P_\ell(x) = (-1)^\ell \binom{m}{\ell} \sum_{k=0}^n (-1)^{k(m+1)} \binom{n}{k}^{m+1} x^k \omega_\ell(m+1, -k). \tag{3.2}$$

Then the corresponding residual function satisfies:

$$R_n^m(x) := \sum_{\ell=0}^m {}_m P_\ell(x) \{ \ln x \}^{m-\ell} = \mathcal{O}\left\{ (x-1)^{m+n+mn} \right\}. \tag{3.3}$$

Proof. It is obvious that ${}_m P_0(x)$ satisfies the normalization condition ${}_m P_0(0) = 1$.

Let δ_x stand for the differential operator $\delta_x = x\mathcal{D}_x$. In order to show that

$$\mathcal{D}_x^\theta R_n^m(x) \Big|_{x=1} = 0 \quad \text{for } 0 \leq \theta < m + n + mn$$

it suffices to check that

$$\delta_x^\theta R_n^m(x) \Big|_{x=1} = 0 \quad \text{for } 0 \leq \theta < m + n + mn$$

thanks to the Stirling inversion formulae [4, p. 220]:

$$x^n D_x^n = \sum_{k=1}^n s(n, k) (x D_x)^k, \tag{3.4a}$$

$$(x D_x)^n = \sum_{k=1}^n S(n, k) x^k D^k. \tag{3.4b}$$

Substituting $\{ {}_m P_\ell(x) \}$ into $R_n^m(x)$, we can reformulate the residual function as

$$R_n^m(x) = \sum_{\ell=0}^m (-1)^\ell \binom{m}{\ell} \{\ln x\}^{m-\ell} \sum_{k=0}^n (-1)^{k(m+1)} \binom{n}{k}^{m+1} x^k \omega_\ell(m+1, -k) \tag{3.5a}$$

$$= \sum_{k=0}^n (-1)^{k+m+km} \binom{n}{k}^{m+1} x^k \sum_{\ell=0}^m (-1)^\ell \binom{m}{\ell} \omega_{m-\ell}(m+1, -k) \{\ln x\}^\ell. \tag{3.5b}$$

By means of the Leibniz rule, it is not hard to verify

$$\delta_x^\ell x^k \Big|_{x=1} = k^\ell \quad \text{and} \quad \delta_x^j \{\ln x\}^\ell \Big|_{x=1} = \begin{cases} \ell!, & j = \ell, \\ 0, & j \neq \ell. \end{cases}$$

They allow us to compute the following derivatives of higher order

$$\delta_x^\theta x^k \{\ln x\}^\ell \Big|_{x=1} = \ell! \binom{\theta}{\ell} k^{\theta-\ell} \tag{3.6}$$

which leads us to the following:

$$\begin{aligned} \delta_x^\theta R_n^m(x) \Big|_{x=1} &= (-1)^m \sum_{k=0}^n (-1)^{k(m+1)} \binom{n}{k}^{m+1} \\ &\quad \times \sum_{\ell=0}^m (-1)^\ell \binom{m}{\ell} \omega_{m-\ell}(m+1, -k) \delta_x^\theta x^k \{\ln x\}^\ell \Big|_{x=1} \\ &= (-1)^{m+\theta} \sum_{k=0}^n (-1)^{k(m+1)} \binom{n}{k}^{m+1} \\ &\quad \times \sum_{\ell=0}^{\theta} (-k)^{\theta-\ell} \binom{\theta}{\ell} \binom{m}{\ell} \ell! \omega_{m-\ell}(m+1, -k). \end{aligned}$$

In view of relation (2.3), the last expression can be restated as

$$\delta_x^\theta R_n^m(x) \Big|_{x=1} = (-1)^{m+\theta} \sum_{k=0}^n (-1)^{k(m+1)} \binom{n}{k}^{m+1} \Omega_m(m+1, \theta, -k) \tag{3.7}$$

which vanishes for $0 \leq \theta < m + n + mn$ thanks to Corollary 7. \square

According to (1.6a) and the Leibniz rule, we can rewrite the sum with respect to ℓ displayed in (3.5b) as

$$\sum_{\ell=0}^m (-1)^\ell \binom{m}{\ell} \omega_{m-\ell}(m+1, -k) \{\ln x\}^\ell = \frac{\mathcal{D}_z^m \{x^{-z} h^{m+1}(z)\}}{x^k h^{m+1}(z)} \Big|_{z=-k}.$$

For a positive real number ε with $0 < \varepsilon < 1$, we can further express the numerator in terms of the Cauchy integral as

$$\begin{aligned} \mathcal{D}_z^m \{x^{-z} h^{m+1}(z)\} \Big|_{z=-k} &= \frac{m!}{2\pi i} \oint_{|z+k|=\varepsilon} \frac{h^{m+1}(z)}{(z+k)^{m+1}} \frac{dz}{x^z} \\ &= \frac{m!}{2\pi i} \oint_{|z+k|=\varepsilon} \frac{(n!)^{m+1} dz}{(z)_{n+1}^{m+1} x^z}. \end{aligned}$$

Substituting them into (3.5b) and then applying the residue theorem, we derive the following integral representation for the residual function (3.3).

Corollary 9. *The residual function of the Padé approximation to the logarithm is equal to the contour integral*

$$R_n^m(x) = (-1)^m (n!)^{m+1} \frac{m!}{2\pi i} \oint_C \frac{dz}{x^z (z)_{n+1}^{m+1}}, \tag{3.8}$$

where C is a rectifiable contour which encloses the real interval $[0, n]$.

By combining the integral representation (3.8) and the following Taylor polynomial of order $M = m + n + mn$ for $1/x^z$ at $x = 1$:

$$\frac{1}{x^z} = \sum_{k=0}^{M-1} \binom{-z}{k} (x-1)^k + M \binom{-z}{M} \int_1^x \frac{(x-t)^{M-1}}{t^{z+M}} dt \tag{3.9}$$

one can obtain an alternative demonstration of (3.3). The details will not be reproduced here.

Remark. The generalized Hermite–Padé approximants ${}_m P_\ell(x)$ may admit different expressions. For example, Driver et al. (DPSW) have figured out, at the end of their joint paper [6], a double sum expression concerning transcendental number π and higher derivatives of binomial coefficient $\binom{n}{k}^{m+1}$ with respect to k . Formally it is much more complicated than (3.2) for the presence of transcendental number π . However, if we ignore all the terms involving π , then it is not difficult to check that the expression conjectured by DPSW coincides with (3.2). Should their conjecture be true, it would be interesting to verify that the collection of all the terms involving π appeared in their double sum expression results in zero.

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