On asymptotics, Stirling numbers, Gamma function and polylogs

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Dec 2005

Abstract

We apply the Euler–Maclaurin formula to find the asymptotic expansion of the sums $\sum_{k=1}^{n}(\log k)^p/k^q$, $\sum k^q(\log k)^p$, $\sum(\log k)^p/(n-k)^q$, $\sum 1/k^q(\log k)^p$ in closed form to arbitrary order ($p, q \in \mathbb{N}$). The expressions often simplify considerably and the coefficients are recognizable constants. The constant terms of the asymptotics are either $\zeta^{(p)}(\pm q)$ (first two sums), 0 (third sum) or yield novel mathematical constants (fourth sum). This allows numerical computation of $\zeta^{(p)}(\pm q)$ faster than any current software. One of the constants also appears in the expansion of the function $\sum_{n\geqslant 2}(n\log n)^{-s}$ around the singularity at $s = 1$; this requires the asymptotics of the incomplete gamma function. The manipulations involve polylogs for which we find a representation in terms of Nielsen integrals, as well as mysterious conjectures for Bernoulli numbers. Applications include the determination of the asymptotic growth of the Taylor coefficients of $(-z/\log(1-z))^k$. We also give the asymptotics of Stirling numbers of first kind and their formula in terms of harmonic numbers.

1   Introduction

This paper is about concrete mathematics. It gathers several results about asymptotic theory, half of which are obtained from the Euler–Maclaurin formula. A few by-products offer themselves, such as the asymptotics of the incomplete gamma function, or the study of the complex function $\sum_{n \geqslant 2}(n \log n)^{-s}$ with a singularity at $s = 1$, or representations of polylogs in terms of Nielsen integrals, or properties of Stirling numbers, or some identities about Bernoulli numbers. We also summarise three ways of obtaining the asymptotic growth of the Taylor coefficients of $(-z/\log(1-z))^k$. Much of the contents may not be new – let alone ground-breaking, but the interest of the paper lies in the way all these objects tie the knot and pop up by studying a few simple problems; it will offer some surprises to the curious and hands-on mathematician.

To begin with, we recall the Euler–Maclaurin formula:

$$\sum_{k=a}^{n-1} f(k) = \int_a^n f(x)dx - \tfrac{1}{2}[f(n) - f(a)] + \sum_{k=1}^m \frac{B_{2k}}{(2k)!}[f^{(2k-1)}(n) - f^{(2k-1)}(a)] + \text{error}$$

where the error term is $O(\frac{1}{(2\pi)^{2m}}) \int_a^n |f^{(2m)}(x)|dx$. The values of $\frac{B_{2k}}{(2k)!}$ are $\frac{1}{12}, -\frac{1}{720}, \frac{1}{30240}, \dots$.

We shall be interested in the limit of large n, keeping a fixed. When ordering the terms in decreasing orders of n, the quantity $-\sum_{k=1}^m \frac{B_{2k}}{(2k)!} f^{(2k-1)}(a)$ will contribute to the constant term. The constant term will be exact when all orders have been taken into account (ie. $m \to \infty$). Since this means adding always bigger chunks ($B_{2k} \sim (2k)^{2k}$), we would end up with an infinite value for the constant term. In practice, the exact value of the constant term has to be computed from another approach. However, the formal infinite sum involving Bernoulli numbers appears most useful, as it behaves linearly: adding two such sums (from the asymptotics of H_n and $H_n^{(2)}$, say) will stand for a constant whose exact value is the sum of the two exact values of the respective constant terms.

We shall use this trick in <u>section 2</u> to write down the exact constants hiding behind formal sums. They will prove useful in subsequent sections to derive the coefficients in the asymptotic expansions (for large n) of the four sums that we consider in sections 4,5,6,7 respectively:

$$\sum_{k=1}^n \frac{(\log k)^p}{k^q}, \qquad \sum_{k=1}^n k^q (\log k)^p, \qquad \sum_{k=1}^{n-1} \frac{(\log k)^p}{(n-k)^q}, \qquad \sum_{k=2}^{n-1} \frac{1}{k^q (\log k)^p}$$

for $p, q \in \mathbb{N}$. We shall write their asymptotics in closed form to arbitrary order of n. In particular, we can write down $\zeta^{(p)}(\pm q)$ and the Stieltjes constants γ_p as formal sums over rational numbers. In this formal sense, $\gamma_p = (-1)^p \zeta^{(p)}(1)$.

The coefficients in the asymptotic expansions often contain Stirling numbers of the first kind, or their close relative which we denote by $S_{r,s,t} := \sum \frac{1}{i_1 \cdots i_r}$ (sum over all integers i_j such that $s \leqslant i_1 < \dots < i_r \leqslant t$). <u>Section 3</u> expresses these numbers in terms of harmonic numbers, which allows a rapid deduction of their asymptotics to arbitrary order. The formula can be inverted to express harmonic numbers in terms of Stirling numbers.

The asymptotic expansion of the four sums, presented in <u>sections 4,5,6,7</u>, can be easily derived from the Euler–Maclaurin formula for the first two sums but involves intricate algebra for the latter two. In those cases, the expansion was first found empirically using the asymp_k trick (appendix). The coefficients are all rational numbers except for the constant terms ($\zeta^{(p)}(\pm q)$ for the first two sums, unknown constants for the fourth sum). For the third sum, the constant term vanishes but $\zeta^{(p)}(-q)$ occurs at higher orders (irrational). The asymp_k trick gives us sufficient digits of a coefficient c; we then can use the PARI software to find a vanishing integer linear combination of $1, c, \zeta'(7)$, say, if one suspected there was a $\zeta'(7)$ hiding behind c. The proper linear combination requires often guesswork. As an application, knowing a large number of terms of the asymptotic expansion of the first two sums allows one to compute the constant term $\zeta^{(p)}(\pm q)$ to arbitrary precision more rapidly than any current mathematical software; the asymp_k trick can also enhance speed.

As an application, we derive in <u>section 8</u> the asymptotic growth of the coefficients in the Taylor expansion of $(-z/\log(1-z))^k$, via a convolution from the ansatz at $k = 1$ (the latter known to Pólya). The result appeared in two other contexts ([N-61] and [FO-90]) which we recapitulate for the interested reader.

As advertised, the fourth sum (section 7) gives birth to a 2d-array of unknown mathematical constants, $C_{p,q}$, that converge to the values of $1/(2^q(\log 2)^p)$ when $p, q \to \infty$; only $C_{1,0}$ and $C_{1,1}$ have appeared (indirectly) before in the literature. <u>Section 9</u> verifies that $C_{1,1}$, which occurs in $\sum_{k=1}^{n} \frac{1}{k \log k} \approx \log \log n + C_{1,1} + O(\frac{1}{n \log n})$, also occurs in the constant term of the asymptotic expansion of the following complex function around its singularity at $s = 1$:

$$\sum_{n=2}^{\infty} \frac{1}{(n \log n)^s} \approx -\log(s-1) + C_{1,1} - \gamma + O\big((s-1)\log^2(s-1)\big) \qquad \text{as} \;\; s \to 1.$$

This involves the asymptotics of the incomplete gamma function.

In order to prove the asymptotic expansion of the third sum (section 6) via the Euler–Maclaurin formula, one needs to track down surprising cancellations. The manipulations involve a particular representation of polylogs by Nielsen integrals $\mathfrak{S}_{1,p}(x)$ presented in <u>section 10</u>:

$$\mathrm{Li}_j(1-x) = \sum_{r=0}^{j-1} \Big(\zeta(j-r) - \mathfrak{S}_{1,j-r-1}(x)\Big) \frac{\log^r(1-x)}{r!},$$

wherein the term with $\zeta(1)$ should be dropped. The generalised polylogs $\mathrm{Li}_{s_1,\ldots,s_k}(x) := \sum \frac{x^{n_1}}{n_1^{s_1}\ldots n_k^{s_k}}$ (sum over integers n_j with $n_1 > \cdots > n_k > 0$) give rise to the Nielsen integrals: $\mathfrak{S}_{k,p}(x) = \mathrm{Li}_{k+1,1^{p-1}}(x)$ (the subscript 1^{p-1} stands for $p-1$ times 1). Thus, the representation can be rewritten as

$$\mathrm{Li}_j(1-x) = \sum_{r=0}^{j-1} \Big(\mathrm{Li}_{j-r}(1) - \mathrm{Li}_{2,1^{j-r-2}}(x)\Big)(-1)^r \, \mathrm{Li}_{1^r}(x),$$

wherein the term with $\mathrm{Li}_1(1)$ should be dropped. Proving the asymptotics of the third sum for $p = 2$ entails two curious representations of Nielsen integrals, (10.9) and (10.10), which themselves boil down

to the following bizarre identities for Bernoulli numbers: For n a positive integer, $n \geqslant 2$,

$$\sum_{r=1}^{n-1} \frac{(-1)^r B_r}{r} \sum_{l=r}^{n} \frac{(-1)^l}{l} \binom{n-1}{n-l} = -\frac{1}{n^2}$$

$$\sum_{r=1}^{n-1} \frac{(-1)^r B_r}{r} \Big(\sum_{l=r}^{n} (-1)^l \binom{n}{l} H_{l-1} + \frac{1}{r} + \frac{1}{n-r} \Big) = H_{n-1}^{(2)} + \frac{1}{n} H_{n-1}.$$

Proving the asymptotics for higher p, one gets a further such identity, and a whole tower can be built up. The first identity is easy to prove, but the second has resisted our best efforts (and those of experts).

2 Formal sums of Bernoulli numbers and zeta-values

We start with formal infinite sums involving Bernoulli numbers. The notation is formal because the sums diverge $(B_{2k} \sim (2k)^{2k})$. Nevertheless, they are useful as one can recognize constant terms from the expressions $\sum \frac{B_{2k}}{(2k)!} c_k$ in the Euler–Maclaurin formula. We shall use such (diverging) expressions to recognize constants in future applications of the Euler–Maclaurin formula.

Lemma 2.1. *In formal notation:*

$$\gamma = \tfrac{1}{2} + \sum_1 \frac{B_{2k}}{2k} \tag{2.2}$$

$$\zeta(2) = \tfrac{3}{2} + \sum B_{2k} \tag{2.3}$$

$$\zeta(3) = 1 + \sum B_{2k} \frac{2k+1}{2} \tag{2.4}$$

$$\zeta(4) = \tfrac{5}{6} + \sum B_{2k} \frac{(2k+1)(2k+2)}{2 \cdot 3} \tag{2.5}$$

$$\zeta(i) = \frac{i+1}{2i-2} + \sum \frac{B_{2k}}{(2k)!} \frac{(2k+i-2)!}{(i-1)!} \tag{2.6}$$

$$\tfrac{1}{2} \log(2\pi) = -\zeta'(0) = 1 - \sum \frac{B_{2k}}{(2k)(2k-1)} \tag{2.7}$$

$$\tfrac{1}{12} - \zeta'(-1) = \tfrac{1}{4} + \sum_2 \frac{B_{2k}}{(2k)(2k-1)(2k-2)} \tag{2.8}$$

$$-\zeta'(-2) = \tfrac{1}{36} - 2! \sum_2 \frac{B_{2k}}{(2k)\ldots(2k-3)} \tag{2.9}$$

$$-\tfrac{11}{720} - \zeta'(-3) = -\tfrac{1}{48} + 3! \sum_3 \frac{B_{2k}}{(2k)\ldots(2k-4)} \tag{2.10}$$

$$\frac{B_{q+1}}{q+1} H_q - \zeta'(-q) = \frac{1}{(q+1)^2} - \sum_{k=1}^{\lfloor \frac{q}{2} \rfloor} \frac{B_{2k}}{(2k)!} \frac{q! \ (H_q - H_{q-2k+1})}{(q-2k+1)!} - (-1)^q q! \sum_{k \geqslant \lceil \frac{q}{2} \rceil + 1} \frac{B_{2k}}{(2k)\ldots(2k-q-1)} \tag{2.11}$$

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$$\sum_1 \frac{B_{2k}}{2k} = \gamma - \tfrac{1}{2} \tag{2.12}$$

$$\sum_1 \frac{B_{2k}}{2k-1} = \zeta'(0) + \gamma + \tfrac{1}{2} = -\tfrac{1}{2}\log(2\pi) + \gamma + \tfrac{1}{2} \tag{2.13}$$

$$\sum_2 \frac{B_{2k}}{2k-2} = -2\zeta'(-1) + 2\zeta'(0) + \gamma + \tfrac{11}{12} \tag{2.14}$$

$$\sum_2 \frac{B_{2k}}{2k-3} = 3\zeta'(-2) - 6\zeta'(-1) + 3\zeta'(0) + \gamma + \tfrac{5}{4} \tag{2.15}$$

$$\sum_{\lfloor \frac{j}{2}\rfloor+1} \frac{B_{2k}}{2k-j} = \sum_{i=1}^{j}(-1)^{i+j}i\binom{j}{i}\zeta'(i-j) + \gamma + \left(H_j - \tfrac{1}{2} - \sum_{k=1}^{\lfloor\frac{j}{2}\rfloor}\frac{B_{2k}}{2k}\right), \qquad (j \geqslant 0) \tag{2.16}$$

$$\sum_{\lfloor \frac{j}{2}\rfloor+1} \frac{B_{2k}}{(2k)(2k-j)} = \sum_{i=1}^{j}(-1)^{i+j}\binom{j-1}{i-1}\zeta'(i-j) + \frac{H_j}{j}, \qquad (j \geqslant 1) \tag{2.17}$$

$$\sum B_{2k}\frac{2k-1}{2} = \zeta(3) - \zeta(2) + \tfrac{1}{2} \tag{2.18}$$

$$\sum \frac{B_{2k}(2k-2)}{2k(2k-1)} = \gamma - \tfrac{3}{2} + \tfrac{1}{2}\log(2\pi) \tag{2.19}$$

$$H_n = \log n + \gamma + \frac{1}{2n} - \sum_1^m \frac{B_{2k}}{2k}\frac{1}{n^{2k}} + O\left(\tfrac{1}{n^{2m+1}}\right) \tag{2.20}$$

$$(i \geqslant 2 :) \qquad H_n^{(i)} = \zeta(i) - \frac{1}{(i-1)n^{i-1}} + \frac{1}{2n^i} - \sum_1^m \frac{B_{2k}}{(2k)!}\frac{(i+2k-2)!}{(i-1)!}\frac{1}{n^{i+2k-1}} + O\left(\tfrac{1}{n^{i+2m}}\right) \tag{2.21}$$

Proof. The first five lines are the constant terms in the asymptotic expansion of $H_n, H_n^{(2)}, H_n^{(3)}, H_n^{(4)}, H_n^{(i)}$. The next five lines are the constant terms in the asymptotic expansion of $\sum^n k^q \log k$ $(q = 0, 1, 2, 3)$, the first being given by the Stirling formula (for $\log n!$). These are the generalized Glaisher constants [F-03], see lemma 5.2. The third set of lines is obtained recursively by partial fraction decomposition from the previous: $\frac{1}{2k-j} = \frac{j!}{(2k)...(2k-j)} - \sum_{i=0}^{j-1}\frac{(-1)^{i+j}\binom{j}{i}}{2k-i}$; while we used $\frac{1}{(2k)(2k-j)} = -\frac{1}{j}(\frac{1}{2k} - \frac{1}{2k-j})$ for (2.17). Lines (2.18) and (2.19) are miscellaneous linear combinations that we shall use. The last two lines yield the asymptotics for the generalized harmonic numbers $\sum_{k=1}^n \frac{1}{k^i}$, with $\zeta(i)$ in (2.6) as it appears in the Euler–Maclaurin formula. $\qquad\square$

Lemma 2.22.

$$\sum_1 \frac{B_{2k}}{2k}\frac{(2k)\cdots(2k+i-2)}{(i-1)!} = \zeta(i) - \frac{i+1}{2i-2} \tag{2.23}$$

$$\sum \frac{B_{2k}}{2k}\frac{(2k-1)\cdots(2k+i-3)}{(i-1)!} = \zeta(i) - \zeta(i-1) + \frac{1}{(i-1)(i-2)} \tag{2.24}$$

$$\sum \frac{B_{2k}}{2k}\frac{(2k-j)\cdots(2k+i-2-j)}{(i-1)!} = \sum_{r=0}^{j}(-1)^r\binom{j}{r}\zeta(i-r) + \frac{(-1)^{j+1}\,j!}{(i-1)\cdots(i-j-1)}, \qquad (1 \leqslant j \leqslant i-2) \tag{2.25}$$

$$= \sum_{r=0}^{i-1}(-1)^r\binom{j}{r}\zeta(i-r) + c_{j,i}, \qquad (j \geqslant i-1, \; i \geqslant 2) \tag{2.26}$$

$$= \sum_{r=0}^{i-1}\binom{-j-1+r}{r}\zeta(i-r) + c_{j,i}, \qquad (j \leqslant -1, \; i \geqslant 2) \tag{2.27}$$

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with $\zeta(1)$ standing for Euler's γ in the last two equations. As to the constants, they are computed recursively, $\forall j \in \mathbb{Z}, i \geqslant 2$:

$c_{j,i} = c_{j-1,i} - c_{j-1,i-1}$, hence $c_{j,i} = (-1)^{i+1}\left(\sum_{r=3}^{i}(-1)^r c_{j-i-1+r,r} - c_{j-i+2,2}\right)$, which is useful for the fourth line; while $c_{j,i} = c_{j+1,i-1} - c_{j,i-1}$, hence $c_{j,i} = \sum_{r=3}^{i} c_{j+1,r} - c_{j,2}$, is useful for the fifth line. The third line can be used for values of $c_{j,i}$ with $1 \leqslant j \leqslant i-2$. For any j: $c_{j,2} = \frac{i-3}{2}$.

For instance: $c_{i-2,i} = \frac{(-1)^{i-1}}{i-1}$ $(i \geqslant 3$, and $c_{0,2} = -\frac{3}{2})$, and $c_{i-1,i} = (-1)^{i-1}H_{i-1}$ $(i \geqslant 2)$.

Proof. These are direct combinatorial consequences of (2.6). $\qquad\square$

In the lhs of the fourth line $(j \geqslant i-1)$, one can choose to exclude the few non-zero terms at low values of k; in that case $\sum_1$ is replaced by $\sum_{\lceil \frac{i-i}{2} \rceil}$ and the only change lies in the constants: $c_{j,2} = \frac{j-3}{2} - \sum_{k=1}^{\lceil \frac{j}{2} \rceil - 1} B_{2k}\left(1 - \frac{j}{2k}\right)$, and the recursions remain unchanged.

3 Stirling numbers and their asymptotics

For future use, we set

$$\boxed{S_{r,s,t} := \sum_{s \leqslant i_1 < \cdots < i_r \leqslant t} \frac{1}{i_1 \cdots i_r}},$$

which is 0 for $t < r + s - 1$. Define $S_{0,s,t} := 1$ if $t \geqslant s - 1$ and $S_{r,s,t} := 0$ if $r < 0$. These numbers relate to the Stirling numbers of the first kind $\begin{bmatrix} t \\ r \end{bmatrix}$, defined by $\sum_k \begin{bmatrix} n \\ k \end{bmatrix} x^k := x(x+1)\cdots(x+n-1)$, or to the *signed* Stirling numbers $s(t,r)$, defined by $\sum_k s(n,k)x^k := x(x-1)\cdots(x-n+1)$, in the following way: $S_{r,1,t} = \begin{bmatrix} t+1 \\ r+1 \end{bmatrix}/t! = (-1)^{r+t}s(t+1,r+1)/t!$. The generating function for these three versions are:

$$\frac{1}{r!}(\log(1+x))^r = \sum_{n \geqslant 1} s(n,r)\frac{x^n}{n!}$$

$$\frac{1}{r!}(-\log(1-x))^r = \sum_{n \geqslant 1} \begin{bmatrix} n \\ r \end{bmatrix}\frac{x^n}{n!}$$

$$\frac{1}{r!}(-\log(1-x))^r = \sum_{n \geqslant 1} S_{r-1,1,n-1}\frac{x^n}{n}.$$

Here is the relation between Stirling numbers of the first kind and harmonic numbers. Denote by $\{r\} = r_1^{i_1}\ldots r_l^{i_l}$ a partition of the integer r into l different parts, ie $r = i_1 r_1 + \cdots + i_l r_l$. Then:

$$S_{r,1,n} = (-1)^r \sum_{\{r\}} \prod_{j=1}^{l} \frac{(-1)^{i_j}}{i_j!}\left(\frac{H_n^{(r_j)}}{r_j}\right)^{i_j}. \tag{3.1}$$

The first few cases are $S_{1,1,n} = H_n$ (partition $\{1\}=1$), and:

$S_{2,1,n} = -\frac{1}{2}H_n^{(2)} + \frac{1}{2}H_n^2$ partitions $\{2\} = 2, 1^2$.

$S_{3,1,n} = \frac{1}{3}H_n^{(3)} - \frac{1}{2}H_n^{(2)}H_n + \frac{1}{6}H_n^3$ partitions $\{3\} = 3, 21, 1^3$.

$S_{4,1,n} = -\frac{1}{4}H_n^{(4)} + \frac{1}{3}H_n^{(3)}H_n + \frac{1}{8}(H_n^{(2)})^2 - \frac{1}{4}H_n^{(2)}H_n^2 + \frac{1}{24}H_n^4$ partitions $\{4\} = 4, 31, 2^2, 21^2, 1^4$.

This can be used, in combination with (2.20) and (2.21), to compute the asymptotic growth of the Stirling numbers to arbitrary order. The terms contributing the most are those with highest power of H_n ($\sim \log n$): partitions $\{r\} = 1^r, 21^{r-2}$, etc. Thus the asymptotic expansion starts as

$$S_{r,1,n} = \frac{1}{r!}(\log n)^r + \frac{\gamma}{(r-1)!}(\log n)^{r-1} + \frac{\gamma^2 - \zeta(2)}{(r-2)!\, 2}(\log n)^{r-2} + \dots \qquad \text{for fixed } r \qquad (3.2)$$

For an alternative proof of this result and for shedding light on the decreasing sequence of logarithms, see end of section 6. Equation (3.2) is the main result of [W-93] and was strengthened in [H-95].

As for the asymptotic behaviour when r grows as quickly as n, say for $n - r$ fixed, formula (3.1) is helpless; but we can easily find the solution by intuition: $n! S_{n,1,n} = 1$, $n! S_{n-1,1,n} = 1 + \cdots + n = n(n+1)/2$, $n! S_{n-2,1,n} = \sum_{i_1=1}^n \sum_{i_2=i_1+1}^n i_1 i_2 = \frac{1}{2}\,(\text{square} - \text{diag}) = \frac{1}{2}[n^2(n+1)^2/4 - n(n+1)(2n+1)/6] = n(n+1)(3n^2 - n - 2)/24 \sim n^4/8$. Similarly: $n! S_{n-3,1,n} = \sum_{i_1=1}^n \sum_{i_2=i_1+1}^n \sum_{i_3=i_2+1}^n i_1 i_2 i_3 = \frac{1}{3!}\,(\text{cube} - \text{plane}) \sim \frac{1}{3!}(n(n+1)/2)^3$; and in general we will have $n! S_{n-k,1,n} \sim \frac{1}{k!}(n(n+1)/2)^k$, that is:

$$S_{r,1,n} = \frac{1}{n!}\frac{1}{(n-r)!}\left(\frac{n^2}{2}\right)^{n-r} + \dots \qquad \text{for } n - r \text{ const.}$$

These two asymptotic growths agree with the results of [MW-58] obtained by saddle-point evaluation of the generating function integral (a method already used by Laplace two centuries ago for Stirling numbers of second kind). The same results were re-obtained in [KK-91] from recursion equations using the ray method from optics. Formula (3.1), however, gives as many terms as desired for the growth with r fixed.

Formula (3.1) can be inverted to yield

$$H_n^{(r)} = (-1)^r r \sum_{\{r\}} (-1)^{i_1 + \cdots + i_l} \frac{(i_1 + \cdots + i_l - 1)!}{i_1! \cdots i_l!}\, S_{r_1,1,n}^{i_1} \cdots S_{r_l,1,n}^{i_l}.$$

4 Asymptotics of sums involving $(\log k)^p / k^q$

Lemma 4.1. $\sum_{k=1}^n \frac{\log k}{k} = (\log n)\left[H_n - \frac{1}{2}\log n - \gamma\right] + \gamma_1 + \sum_{k=1}^m \frac{B_{2k} H_{2k-1}}{(2k)\, n^{2k}} + O(\frac{1}{n^{2m+1}})$, with $\gamma_1 = -\sum \frac{B_{2k}}{2k} H_{2k-1}$.

Proof. Write the lhs as $\frac{\log n}{n} + \sum_{k=1}^{n-1} \frac{\log(k)}{k}$. For $f(x) := \frac{\log x}{x}$, here are the ingredients we need: $\int f(x) = \frac{(\log x)^2}{2}$, $f^{(2k-1)}(x) = (2k-1)! \frac{H_{2k-1} - \log x}{x^{2k}}$. Thus the Euler–Maclaurin formula tells us that $\sum_{k=1}^{n-1} \frac{\log(k)}{k} = \frac{(\log n)^2}{2} - \frac{1}{2}\frac{\log n}{n} + \sum \frac{B_{2k}}{(2k)n^{2k}}(H_{2k-1} - \log n) - \sum \frac{B_{2k} H_{2k-1}}{(2k)}$. The $\log n$ terms yield $-(\log n)\sum \frac{B_{2k}}{(2k)n^{2k}}$, which estimates $(\log n)[H_n - \gamma - \frac{1}{2n}]$ by (2.20). Writing $(\log n)\left[H_n - \frac{1}{2}\log n - \gamma\right]$ assures us that the remaining terms are inverse powers of n (easily tractable under the asymp_k trick). The constant γ_1 is by definition the first Stieltjes constant. $\qquad \square$

Using the same method of proof, we easily generalise.

Lemma 4.2. $\sum_{k=1}^n \frac{(\log k)^2}{k} = \frac{(\log n)^3}{3} + \gamma_2 + \frac{1}{2}\frac{(\log n)^2}{n} - \sum_{k=1}^m \frac{B_{2k}}{2k}\frac{(\log n)^2 - 2H_{2k-1}(\log n) + H_{2k-1}^2 - H_{2k-1}^{(2)}}{n^{2k}} + O(\frac{(\log n)^2}{n^{2m+1}})$, with $\gamma_2 = \sum \frac{B_{2k}(H_{2k-1}^2 - H_{2k-1}^{(2)})}{2k}$. Similarly, for $p \geqslant 0$:

$$\sum_{k=1}^n \frac{(\log k)^p}{k} = \frac{1}{p+1}(\log n)^{p+1} + \gamma_p + \frac{1}{2}\frac{(\log n)^p}{n} - \sum_{k=1}^m \frac{\sum_{r=0}^p d_{p,k,r}(\log n)^{p-r}}{n^{2k}} + O(\frac{(\log n)^p}{n^{2m+1}}),$$

with $d_{p,k,r} = \frac{B_{2k}}{2k} \frac{(-1)^r p!}{(p-r)!} \; S_{r,1,2k-1}$ $\quad$ and $\gamma_p = (-1)^p \; p! \sum_{k>p/2} \frac{B_{2k}}{2k} \; S_{p,1,2k-1}$.

Here, γ_p is the p-th Stieltjes constant by definition. For $p = 0$ we have $S_{0,s,t} = 1$ and $\gamma_0 = \gamma$ (though one needs to add $\frac{1}{2}$ to γ_p in this case). Note that in the last sum, we could drop the requirement $k > p/2$, as $S_{p,1,2k-1}$ vanishes for $k = 1, \ldots, p/2$. We will neglect this in future.

Note that the expressions we find for γ_p are exactly the same as those one finds when directly analytically expanding the zeta function via the Euler–Maclaurin formula. One uses $f(x) := x^{-s}$ with

$$f^{(2k-1)}(x) = -s(s+1)\cdots(s+2k-2)\; x^{-s-2k+1} = -(2k-1)! \; \sum_{p=0}^{2k-1} S_{p,1,2k-1}(s-1)^p \; x^{-s-2k+1}:$$

$$\zeta(s) = \lim_{N\to\infty} \sum_{n=1}^{N} \frac{1}{n^s} = \frac{1}{s-1} + \tfrac{1}{2} + \sum_{k=1}^{M} \frac{B_{2k}}{(2k)!} \; s(s+1)\cdots(s+2k-2) + \mathrm{error}(s,M)$$

$$= \frac{1}{s-1} + \sum_{p\geqslant 0} \Big(\underbrace{\sum_{k>p/2} \frac{B_{2k}}{2k} S_{p,1,2k-1}}_{\frac{(-1)^p}{p!} \; \gamma_p} \Big)(s-1)^p.$$

We also easily generalise in another direction:

Lemma 4.3. $\sum_{k=1}^{n} \frac{\log k}{k^2} = -\zeta'(2) + (\log n)\big[H_n^{(2)} - \zeta(2)\big] - \frac{1}{n} + \sum_{k=1}^{m} \frac{B_{2k}(H_{2k}-1)}{n^{2k+1}} + O(\frac{1}{n^{2m+2}})$,

with $-\zeta'(2) = 1 - \sum B_{2k}(H_{2k}-1)$. Similarly, for $q \geqslant 2$:

$$\sum_{k=1}^{n} \frac{\log k}{k^q} = -\zeta'(q) + (\log n)\big[H_n^{(q)} - \zeta(q)\big] - \frac{1}{(q-1)^2 n^{q-1}} + \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} \frac{(q+2k-2)!}{(q-1)!} \frac{H_{q+2k-2} - H_{q-1}}{n^{q+2k-1}} + O(\frac{1}{n^{q+2m}}),$$

with $-\zeta'(q) = \frac{1}{(q-1)^2} - \sum \frac{B_{2k}}{(2k)!} \frac{(2k+q-2)!}{(q-1)!}(H_{2k+q-2} - H_{q-1})$.

The meta-generalisation regroups the two previous results:

Lemma 4.4. For $q \geqslant 2$ and $p \geqslant 0$:

$$\sum_{k=1}^{n} \frac{(\log k)^p}{k^q} = (-1)^p \zeta^{(p)}(q) - \frac{\sum_{r=0}^{p} \frac{p!/(p-r)!}{(q-1)^{r+1}}(\log n)^{p-r}}{n^{q-1}} + \frac{1}{2} \frac{(\log n)^p}{n^q} - \sum_{k=1}^{m} \frac{\sum_{r=0}^{p} d_{p,q,k,r}(\log n)^{p-r}}{n^{q+2k-1}} + O(\frac{(\log n)^p}{n^{q+2m}})$$

with $d_{p,q,k,r} = \frac{B_{2k}}{(2k)!} \frac{(2k+q-2)!}{(q-1)!} \frac{(-1)^r p!}{(p-r)!} S_{r,q,2k+q-2}$,

and $(-1)^p \zeta^{(p)}(q) = \frac{p!}{(q-1)^{p+1}} + (-1)^p p! \sum_1 \frac{B_{2k}}{(2k)!} \frac{(2k+q-2)!}{(q-1)!} S_{p,q,2k+q-2}$.

Proof. Write the lhs as $\frac{(\log n)^p}{n^q} + \sum_{k=1}^{n-1} \frac{(\log k)^p}{k^q}$. For $f(x) := \frac{(\log x)^p}{x^q}$, here are the ingredients we need: $\int f(x) = -\frac{1}{(q-1)^{r+1} x^{q-1}} \sum_{r=0}^{p} \frac{p!(\log x)^{p-r}}{(p-r)!}$, $f^{(i)}(x) = \frac{1}{x^{q+i}} \frac{(q+i-1)!}{(q-1)!} \sum_{r=0}^{p} \frac{(-1)^{r+i} p!}{(p-r)!} S_{r,q,q+i-1}(\log x)^{p-r}$ (NB: $S_{\ldots} = 0$ for $r > i$). Now simply apply the Euler–Maclaurin formula. $\qquad\square$

Application to numerics of the ζ function. Note that this formula, together with the asymp$_k$ trick, allows a very rapid numerical computation of $\zeta^{(p)}(q)$ (for positive integer q), much more efficient than current mathematical softwares. Lemmas 5.3 or 6.2 provide a formula for negative q.

5 Asymptotics of sums involving $k^q(\log k)^p$

Lemma 5.1. *For $p \geqslant 1$ we have:*

$$\sum_{k=1}^{n}(\log k)^p = n\sum_{r=0}^{p}\frac{(-1)^r p!}{(p-r)!}(\log n)^{p-r}+\tfrac{1}{2}(\log n)^p+\text{const}-\sum_{k=1}^{m}\frac{\frac{B_{2k}}{2k(2k-1)}\sum_{r=1}^{p}\frac{(-1)^r p!}{(p-r)!}S_{r-1,1,2k-2}(\log n)^{p-r}}{n^{2k-1}}+\mathcal{O}(\tfrac{(\log n)^{p-1}}{n^{2m}}),$$

with $\text{const} = (-1)^p\zeta^{(p)}(0) = (-1)^p p!\big(-1+\sum_1\frac{B_{2k}}{2k(2k-1)}S_{p-1,1,2k-2}\big)$.

Lemma 5.2. *For $q \geqslant 0$ we have:*

$$\sum_{k=1}^{n}k^q\log k = \frac{n^{q+1}}{q+1}\Big[(\log n) - \tfrac{1}{q+1}\Big] + \tfrac{1}{2}n^q\log n + \sum_{k=1}^{\lceil\frac{q}{2}\rceil}\frac{B_{2k}}{(2k)!}\frac{q!}{(q-2k+1)!}\Big[(\log n) + (H_q - H_{q-2k+1})\Big]\,n^{q-2k+1}$$

$$+ \text{const} + (-1)^q q! \sum_{k=\lceil\frac{q}{2}\rceil+1}^{m}\frac{B_{2k}}{(2k)...(2k-q-1)}\frac{1}{n^{2k-q-1}} + O(\tfrac{1}{n^{2m-q}})$$

with $\text{const} = -\zeta'(-q) + \frac{B_{q+1}}{q+1}H_q = \frac{1}{(q+1)^2} - \sum_{k=1}^{\lfloor\frac{q}{2}\rfloor}\frac{B_{2k}}{(2k)!}\frac{q!(H_q-H_{q-2k+1})}{(q-2k+1)!} - (-1)^q q! \sum_{k\geqslant\lceil\frac{q}{2}\rceil+1}\frac{B_{2k}}{(2k)...(2k-q-1)}$ *being the generalized Glaisher constant of (2.11). For odd q, it is understood that the last term of the sum $\sum_{k=1}^{\lceil\frac{q}{2}\rceil}...$ (with $k = \lceil\frac{q}{2}\rceil$ and independent of n), which equals $\frac{B_{q+1}}{q+1}H_q$, should not be counted as it is already counted in* const.

Again, the meta-generalisation regroups the two previous results:

Lemma 5.3. *For $q \geqslant 0$ and $p \geqslant 1$ we have:*

$$\sum_{k=1}^{n}k^q(\log k)^p = n^{q+1}\sum_{r=0}^{p}\frac{(-1)^r p!}{(p-r)!}\frac{(\log n)^{p-r}}{(q+1)^{r+1}} + \tfrac{1}{2}n^q(\log n)^p + \sum_{k=1}^{\lceil\frac{q}{2}\rceil}\Big(\sum_{r=1}^{p}c_{p,q,k,r}(\log n)^{p-r}\Big)\,n^{q-2k+1}+$$

$$+ \text{const} + \sum_{k=\lceil\frac{q}{2}\rceil+1}^{m}\frac{\sum_{r=1}^{p}d_{p,q,k,r}(\log n)^{p-r}}{n^{2k-q-1}} + O(\tfrac{(\log n)^{p-1}}{n^{2m-q}})$$

with $c_{p,q,k,r} := \frac{B_{2k}}{(2k)!}\frac{q!}{(q-2k+1)!}\frac{p!}{(p-r)!}S_{r,q-2k+2,q}$
and $d_{p,q,k,r} := \frac{B_{2k}(-1)^{r+q+1}}{(2k)...(2k-q-1)}\frac{p!q!}{(p-r)!}\sum_{j=0}^{q}(-1)^j S_{j,1,q}S_{r-j-1,1,2k-q-2}$
and $\text{const} = (-1)^p\zeta^{(p)}(-q) + \frac{B_{q+1}}{q+1}p!S_{p,1,q} = \frac{(-1)^{p+1}p!}{(q+1)^{p+1}} - \sum_{k=1}^{\lfloor\frac{q}{2}\rfloor}c_{p,q,k,p} - \sum_{k\geqslant\lceil\frac{q}{2}\rceil+1}d_{p,q,k,p}$.
For odd q, it is understood that the last term of the sum $\sum_{k=1}^{\lceil\frac{q}{2}\rceil}...$ (with $k = \lceil\frac{q}{2}\rceil$ and $r = p$), which is constant and equals $\frac{B_{q+1}}{q+1}p!S_{p,1,q}$, should not be counted as it is already counted in const.

Proof. Write the lhs as $n^q(\log n)^p + \sum_{k=1}^{n-1}k^q(\log k)^p$. For $f(x) := x^q(\log x)^p$, here are the ingredients we need: $\int f(x) = \frac{x^{q+1}}{(q+1)^{r+1}}\sum_{r=0}^{p}\frac{(-1)^p p!}{(p-r)!}(\log x)^{p-r}$ and

$$f^{(i)}(x) = \begin{cases} \frac{x^{q-i}}{(q-i)!}\sum_{r=0}^{p}\frac{p!}{(p-r)!}(\log x)^{p-r}q!S_{r,q-i+1,q} & \text{for } i \leqslant q, \quad (\text{NB}: S_{...} = 0 \text{ for } r > i) \\ \frac{(i-q-1)!}{x^{i-q}}\sum_{r=0}^{p}\frac{(-1)^{r+q+i}p!}{(p-r)!}(\log x)^{p-r}q!\sum_{j=0}^{q}(-1)^j S_{j,1,q}S_{r-j-1,1,i-q-1} & \text{for } i > q, \end{cases}$$

Now simply apply the Euler–Maclaurin formula. □

6 Asymptotics of sums involving $(\log k)^p/(n-k)^q$

Lemma 6.1. $\sum_{k=1}^{n-1} \frac{\log k}{n-k} = (\log n)^2 + \gamma(\log n) - \zeta(2) + \sum_{k=1}^{m} \left(\frac{(-1)^k B_k}{k^2} - \zeta'(1-k) \right) \frac{1}{n^k} + O(\frac{1}{n^{m+1}})$.

Proof. Write the lhs as $\log(n-1) + \sum_{k=1}^{n-2} \frac{\log(k)}{n-k}$. The integral of $f(x) := \frac{\log x}{n-x}$ is: $-\log(x)\log(1-\frac{x}{n}) - \text{Li}_2(\frac{x}{n})$, thus[1] $\int_1^{n-1} f(x) = (\log n)^2 - \zeta(2) + 2\text{Li}_2(\frac{1}{n})$. Note also that $f^{(i)}(x) = i! \frac{\log x}{(n-x)^{i+1}} + i! \sum_{r=1}^{i} \frac{(-1)^{r+1}/r}{(n-x)^{i+1-r} x^r}$, so that $[f^{(2k-1)}(x)]_1^{n-1} = (2k-1)! \left[\log(n-1) + \sum_{r=1}^{2k-1} \frac{(-1)^{r+1}}{r} \left(\frac{1}{(n-1)^r} - \frac{1}{(n-1)^{2k-r}} \right) \right]$.
In total:

$$\sum_{k=1}^{n-1} \frac{\log(k)}{n-k} = (\log n)^2 - \zeta(2) + 2\,\text{Li}_2\left(\frac{1}{n}\right) + \gamma \log(n-1) + \frac{1}{(n-1)} \sum_1 \frac{B_{2k}}{2k}\left(1 - \frac{1}{2k-1}\right) - \frac{1}{(n-1)^2} \sum_2 \frac{B_{2k}}{2k}\left(\frac{1}{2} - \frac{1}{2k-2}\right) + \dots$$

$$+ \frac{(-1)^{j+1}}{(n-1)^j} \sum_{\lfloor \frac{j}{2} \rfloor + 1} \frac{B_{2k}}{2k}\left(\frac{1}{j} - \frac{1}{2k-j}\right) + \dots$$

Now use (2.17) as well as the expansions $\log(n-1) = \log n - (\frac{1}{n} + \frac{1}{n^2} + \dots)$ and $\frac{1}{(n-1)^j} = \sum_{i \geqslant 0} \binom{j+i-1}{i-1} \frac{1}{n^{j+i}}$. There are nice cancellations so that only $-\zeta'(1-k)$ survives at power $\frac{1}{n^k}$. $\qquad \square$

Lemma 6.2. *For $p \geqslant 1$ we have:*

$$\sum_{k=1}^{n-1} \frac{(\log k)^p}{n-k} = (\log n)^{p+1} + \gamma(\log n)^p + \sum_{r=1}^{p} c_{p,r}(\log n)^{p-r}$$

$$- \sum_{k=1}^{m} \left(\frac{(-1)^k B_k}{k^2} \sum_{r=1}^{p} d_{p,r,k}(\log n)^{p-r} - (-1)^p \zeta^{(p)}(1-k) \right) \frac{1}{n^k} + \mathcal{O}\left(\frac{(\log n)^{p-1}}{n^{m+1}}\right)$$

with $c_{p,r} := \frac{(-1)^r p!}{(p-r)!} \zeta(r+1)$ and $d_{p,r,k} := \frac{(-1)^r p!}{(p-r)!} S_{r-1,1,k-1}$. Hence, the constant term is $(-1)^p p! \zeta(p+1)$.

Proof. Write the lhs as $\log^p(n-1) + \sum_{k=1}^{n-2} \frac{(\log k)^p}{n-k}$. With $f(x) := \frac{(\log x)^p}{n-x}$, we have:

$$\int f(x) = -\log(1 - \tfrac{x}{n})(\log x)^p + \sum_{r=1}^{p} \frac{(-1)^r p!}{(p-r)!} \text{Li}_{r+1}(\tfrac{x}{n})(\log x)^{p-r}$$

$$\int_1^{n-1} f(x) = \log(n) \log^p(n-1) + \sum_{r=1}^{p} \frac{(-1)^r p!}{(p-r)!} \text{Li}_{r+1}(1 - \tfrac{1}{n}) \log^{p-r}(n-1) - (-1)^p p! \text{Li}_{p+1}(\tfrac{1}{n})$$

$$= \log(n) \log^p(n-1) - \sum_{r=1}^{p} \frac{(-1)^r p!}{(p-r)!} \left(\mathfrak{S}_{1,r}(\tfrac{1}{n}) - \zeta(r+1) \right)(\log n)^{p-r} - (-1)^p p! \text{Li}_{p+1}(\tfrac{1}{n})$$

$$f^{(i)}(x) = i! \frac{(\log x)^p}{(n-x)^{i+1}} + i! \sum_{j=1}^{i} \frac{(-1)^j/j}{(n-x)^{i+1-j} x^j} \sum_{r=1}^{p} \frac{(-1)^r p!}{(p-r)!} S_{r-1,1,j-1}(\log x)^{p-r}$$

$$[f^{(2k-1)}(x)]_1^{n-1} = (2k-1)! \log^p(n-1) + (2k-1)! \sum_{j=1}^{2k-1} \frac{(-1)^j}{(n-1)^j} \left(\sum_{r=1}^{p} \frac{(-1)^r p!}{(p-r)!} \log^{p-r}(n-1) \frac{S_{r-1,1,j-1}}{j} - (-1)^p \frac{S_{p-1,1,2k-j-1}}{2k-j} \right)$$

where we used the notation $\mathfrak{S}_{1,r}(x) := \sum_{n \geqslant 1} \frac{S_{r-1,1,n-1}}{n^2} x^n$ from section 10. In total:

$$\sum_{k=1}^{n-1} \frac{(\log k)^p}{n-k} = \int_1^{n-1} f(x) + \tfrac{1}{2} \log^p(n-1) + (\gamma - \tfrac{1}{2}) \log^p(n-1)$$

$$- \frac{1}{(n-1)} \sum_{k \geqslant 1} \frac{B_{2k}}{2k} \left(\sum_{r=1}^{p} \frac{(-1)^r p!}{(p-r)!} \log^{p-r}(n-1) \frac{S_{r-1,1,0}}{1} - (-1)^p \frac{S_{p-1,1,2k-2}}{2k-1} \right)$$

$$\pm \dots + \frac{(-1)^j}{(n-1)^j} \sum_{k \geqslant \lfloor \frac{j}{2} \rfloor + 1} \frac{B_{2k}}{2k} \left(\sum_{r=1}^{p} \frac{(-1)^r p!}{(p-r)!} \log^{p-r}(n-1) \frac{S_{r-1,1,j-1}}{j} - (-1)^p \frac{S_{p-1,1,2k-j-1}}{2k-j} \right) + \dots$$

---

[1] We have used: $\text{Li}_2(1-x) + \text{Li}_2(x) = -\log(x)\log(1-x) + \zeta(2)$ (proof by derivation).

The remainder of the proof are nice cancellations, which are impossible to prove in the general case; we exhibit here the case $p = 2$ as a pattern for all other cases. For $\underline{p = 2}$ we have:

$$\sum_{k=1}^{n-1} \frac{(\log k)^2}{n-k} = \int_1^{n-1} f(x) + \tfrac{1}{2}\log^2(n-1) + \sum \frac{B_{2k}}{2k}[f^{(2k-1)}(x)]_1^{n-1}$$

$$= (\log n)^3 + 2(\log n)[\mathfrak{S}_{1,1} - \zeta(2)] - 2[\mathfrak{S}_{1,2}(\tfrac{1}{n}) - \zeta(3) + \text{Li}_3(\tfrac{1}{n})] + \tfrac{1}{2}\log^2(n-1)+$$

$$+ (\gamma - \tfrac{1}{2})\log^2(n-1) + \frac{2}{(n-1)}\sum_1 \frac{B_{2k}}{2k}\Big(\log(n-1) + \frac{H_{2k-2}}{2k-1}\Big) - \frac{2}{(n-1)^2}\sum_2 \frac{B_{2k}}{2k}\Big(\frac{\log(n-1)}{2} - \frac{H_1}{2} + \frac{H_{2k-3}}{2k-2}\Big)$$

$$\pm \cdots + \frac{2(-1)^j}{(n-1)^j}\sum_{\lfloor \frac{j}{2}\rfloor+1} \frac{B_{2k}}{2k}\Big(\frac{\log(n-1)}{j} - \frac{H_{j-1}}{j} + \frac{H_{2k-j-1}}{2k-j}\Big) + \cdots$$

Now replace $\sum_{\lfloor \frac{j}{2}\rfloor+1} \frac{B_{2k}}{2k}$ by $\gamma - \tfrac{1}{2} - \sum_{r=1}^{\lfloor \frac{j}{2}\rfloor} \frac{B_{2r}}{2r}$ and set $h_j := 2\sum_{\lfloor \frac{j}{2}\rfloor+1} \frac{B_{2k}}{2k}\frac{H_{2k-j-1}}{2k-j}$. The $(\gamma - \tfrac{1}{2})$ will cancel out due to $\log(1 - \tfrac{1}{n}) = -\log(1 - \tfrac{1}{1-n}) = \sum_{i\geqslant 1} \frac{(-1)^i}{i(n-1)^i}$ (and the squared version of it). Now use (10.9) and (10.10) to simplify the rest and arrive at

$$\sum_{k=1}^{n-1} \frac{(\log k)^2}{n-k} = (\log n)^3 + \gamma(\log n)^2 - 2\zeta(2)(\log n) + 2\zeta(3) + \sum_{k\geqslant 1}\Big[\frac{(-1)^k B_k}{k^2}2(\log n - H_{k-1}) - \frac{2}{k^3} - \sum_{r=1}^k (-1)^r \binom{k-1}{r-1}h_r\Big]\frac{1}{n^k}.$$

Use $\zeta''(-q) = -\frac{2}{(q+1)^3} - \frac{B_{q+1}}{q+1}2S_{2,1,q} - \sum_{k=1}^{\lfloor \frac{q}{2}\rfloor} \frac{B_{2k}}{(2k)!}\frac{q!}{(q-2k+1)!}2S_{2,q-2k+2,q} - \sum_{k\geqslant\lceil \frac{q}{2}\rceil+1} \frac{B_{2k}(-1)^q 2q!}{(2k)\cdots(2k-q-1)}(H_{2k-q-2} - H_q)$ from lemma 5.3 as well as the partial fraction decomposition $\frac{1}{2k(2k-j)} = \sum_{r=1}^j \frac{(j-1)!}{(j-r)!}\frac{1}{(2k)\cdots(2k-r)}$ to show that

$$h_j := 2\sum_{k\geqslant\lfloor \frac{j}{2}\rfloor+1} \frac{B_{2k}}{2k}\frac{H_{2k-j-1}}{2k-j} = -\sum_{r=1}^j(-1)^r\binom{j-1}{r-1}\Big[\zeta''(1-r) + \tfrac{2}{r^3}\Big]$$

or equivalently: $-\sum_{r=1}^k(-1)^r\binom{k-1}{r-1}h_r = \zeta''(1-k) + \tfrac{2}{k^3}$. This completes the proof for $p = 2$. The proofs for $p \geqslant 3$ run similarly. $\qquad\square$

Lemma 6.3. *For $q \geqslant 2$ we have:*

$$\sum_{k=1}^{n-1} \frac{\log k}{(n-k)^q} = \zeta(q)\log n - \sum_{i=1}^{q-2} \frac{\zeta(q-i)}{i\,n^i} - \frac{2\log n + C_{q-1}}{(q-1)\,n^{q-1}} + \sum_{k=1}^m \Big(\frac{(-1)^k B_k}{k(k+q-1)} - \binom{k+q-2}{q-1}\zeta'(1-k)\Big)\frac{1}{n^{k+q-1}} + O\big(\tfrac{1}{n^{m+q}}\big)$$

with $C_q := \gamma - H_q + \tfrac{2}{q}$. Hence, there is no constant term.

Proof. Write the lhs as $\log(n-1) + \sum_{k=1}^{n-2} \frac{\log(k)}{(n-k)^q}$. With $f(x) := \frac{\log x}{(n-x)^q}$, we have:

$$\int f(x) = -\frac{1}{q-1}(\log x)\Big(\frac{1}{x^{q-1}} - \frac{1}{(x-n)^{q-1}}\Big) + \frac{1}{q-1}\frac{\log(n-x)}{n^{q-1}} - \sum_{i=1}^{q-2}\frac{1}{i(q-1)}\frac{1}{n^{q-i-1}(n-x)^i}$$

$$\int_1^{n-1} f(x) = \frac{1}{q-1}\log(n-1) + \sum_{i=1}^{q-2}\frac{1}{(q-1)i}\frac{1}{n^{q-1-i}}\Big(\frac{1}{(n-1)^i} - 1\Big) - \frac{2}{q-1}\frac{\log(n-1)}{n^{q-1}}$$

$$f^{(i)}(x) = \frac{(q-1+i)!}{(q-1)!}\frac{\log x}{(n-x)^{q+i}} + i!\sum_{r=1}^i \frac{\frac{(-1)^{r+1}}{r}\binom{i-r+q-1}{q-1}}{(n-x)^{q+i-r}x^r}$$

$$[f^{(2k-1)}(x)]_1^{n-1} = \frac{(q+2k-2)!}{(q-1)!}\log(n-1) + (2k-1)!\sum_{r=1}^{2k-1}\frac{(-1)^{r+1}}{r}\binom{2k-r+q-2}{q-1}\Big(\frac{1}{(n-1)^r} - \frac{1}{(n-1)^{2k-r+q-1}}\Big).$$

In total:

$$\sum_{k=1}^{n-1} \frac{\log k}{(n-k)^q} = \int_1^{n-1} f(x) + \tfrac{1}{2}\log(n-1) + \log(n-1)\sum_1 \frac{B_{2k}}{(2k)!}\frac{(q+2k-2)!}{(q-1)!}$$

$$+ \frac{1}{n-1}\sum_1 \frac{B_{2k}}{2k}\binom{2k+q-3}{q-1} - \frac{1}{(n-1)^2}\frac{1}{2}\sum_1 \frac{B_{2k}}{2k}\binom{2k+q-4}{q-1} + \cdots + \frac{1}{(n-1)^{q-1}}\frac{(-1)^q}{q-1}\sum_1 \frac{B_{2k}}{2k}\binom{2k-1}{q-1}$$

$$+ \frac{1}{(n-1)^q}\Big[\frac{(-1)^{q+1}}{q}\sum_1 \frac{B_{2k}}{2k}\binom{2k-2}{q-1} - \sum_1 \frac{B_{2k}}{(2k)(2k-1)}\Big] + \cdots$$

$$+ \frac{(-1)^{j+1}}{(n-1)^{q+j}}\Big[\frac{(-1)^q}{q+j}\sum_{\lfloor \frac{j+1}{2}\rfloor+1} \frac{B_{2k}}{2k}\binom{2k-j-2}{q-1} - \binom{j+q-1}{q-1}\sum_{\lfloor \frac{j+1}{2}\rfloor+1} \frac{B_{2k}}{(2k)(2k-j-1)}\Big] + \cdots$$

Now use (2.17), (2.25), as well as the expansions $\log(n-1) = \log n - (\frac{1}{n} + \frac{1}{n^2} + \dots)$ and $\frac{1}{(n-1)^j} = \sum_{i \geqslant 0} \binom{j+i-1}{i-1} \frac{1}{n^{j+i}}$. There are nice cancellations so that only $-\zeta'(1-k)$ survives at power $\frac{1}{n^k}$. $\square$

Note that without going through the proof, one can empirically determine the values of the C_q just using the asymp_k trick: one first uses the trick to quickly determine the 30 first values of C_q, then uses it again to determine the asymptotic growth of those values up to $\mathcal{O}(\frac{1}{n^6})$ and recognizes the growth of harmonic numbers.

Again, the meta-generalisation regroups the two previous results:

Lemma 6.4. *For $q \geqslant 2$ and $p \geqslant 1$ we have:*

$$\sum_{k=1}^{n-1} \frac{(\log k)^p}{(n-k)^q} = \zeta(q)(\log n)^p + \sum_{i=1}^{q-2} \frac{\zeta(q-i)}{i\, n^i} \sum_{r=1}^{i} c_{p,i,r}(\log n)^{p-r} + \frac{1}{(q-1)\, n^{q-1}} \sum_{r=0}^{p} d_{p,q,r}(\log n)^{p-r}$$

$$- \sum_{k=1}^{m} \left(\frac{(-1)^k B_k}{k(k+q-1)} \sum_{r=1}^{p} c_{p,k+q-1,r}(\log n)^{p-r} - (-1)^p \binom{k+q-2}{q-1} \zeta^{(p)}(1-k) \right) \frac{1}{n^{k+q-1}} + O(\frac{(\log n)^{p-1}}{n^{m+q}})$$

with $\quad c_{p,i,r} := \frac{(-r)^r p!}{(p-r)!} S_{r-1,1,i-1}$

and $d_{p,q,r} := \frac{(-r)^r p!}{(p-r)!} \times \begin{cases} D_{r,q} - (p-r)S_{r,1,q-2} + S_{r-1,1,q-2}\, \gamma + \sum_{s=2}^{r} S_{r-s,1,q-2}\, \zeta(s) & \text{for } r = 0, \dots, q-1 \\ \sum_{s=r-q+2}^{r} S_{r-s,1,q-2}\zeta(s) & \text{for } r = q, \dots, p \quad (\text{in case } p \geqslant q), \end{cases}$

wherein $D_{r,q}$ are the rational numbers

$$D_{r,q} := \sum_{r=0}^{p-2} \sum_{j=1}^{q-p+r} \frac{S_{r,1,j-1}}{j} \left(\frac{S_{p-2-r,1,q-j-2}}{j} - \sum_{r=1}^{q-j-2} \frac{\sum_{i=0}^{r-1}(-1)^i S_{i,1,r-1} S_{p-3-r-i,1,q-j-2-r}}{r(r+j)} \right) + \frac{S_{p-1,1,q-2}}{q-1} - S_{p,1,q-2}.$$

In particular, there is no constant term in the asymptotic expansion.

Proof. Write the lhs as $\log^p(n-1) + \sum_{k=1}^{n-2} \frac{(\log k)^p}{(n-k)^q}$. With $f(x) := \frac{(\log x)^p}{(n-x)^q}$, we have:

$$\int f(x) = \frac{(\log x)^p}{(q-1)!} \sum_{j=0}^{q-2} \binom{q-1}{j} \frac{x^{q-j-1}}{n^{q-1}(n-x)^{q-1-j}}$$

$$+ \sum_{k=1}^{p} \frac{(-1)^k p!}{(p-k)!} (\log x)^{p-k} \left(\sum_{j=1}^{q-2} \left(\sum_{r=0}^{j-1} \frac{S_{k-1,r}\, r!(q-r-3)!}{(j-r-1)!(q-j+r)!} \right) \frac{x^{q-1-j}}{n^{q-1}(n-x)^{q-1-j}} + \sum_{j=1}^{k} \frac{S_{j-1,q-2}}{(q-1)n^{q-1}} \mathrm{Li}_{k-j+1}(\frac{x}{n}) \right)$$

$$\int_{1}^{n-1} f(x) = \left[\frac{p!}{(q-1)n^{q-1}} \left(\sum_{l=0}^{p} \frac{(-1)^l}{(p-l)!} \left(-S_{l,1,q-2} + \sum_{j=1}^{q-l-1} d_{q,l,j} n^j + S_{l-1,1,q-2}(\log n) \right) \right. \right.$$

$$\left. + \sum_{l=0}^{p-2} \left(\sum_{r=0}^{l} \frac{(-1)^{r+p}}{r!} S_{l-r,1,q-2} \log^r(n-1) \right) \mathrm{Li}_{p-l}(1-\frac{1}{n}) \right) \bigg] - \left[(-1)^p p! \sum_{j=1}^{p} \frac{S_{j-1,1,q-2}}{(q-1)n^{q-1}} \mathrm{Li}_{p-j+1}(\frac{1}{n}) \right]$$

$$f^{(i)}(x) = \frac{(q-1+i)!}{(q-1)!} \frac{(\log x)^p}{(n-x)^{q+i}} - \sum_{r=1}^{p} \frac{p!(\log x)^{p-r}}{(p-r)!(q-1)!} \sum_{j=1}^{i+1-r} \frac{(-1)^j i!(q+i-j+r)!}{(j+r-1)(i-j-r+1)!} \frac{S_{r-1,1,j+r-2}}{(n-x)^{q+i-r-j+1} x^{r+j-1}}$$

$$[f^{(2k-1)}(x)]_1^{n-1} = \frac{(q+2k-2)! \log^p(n-1)}{(q-1)!} - \frac{(2k-1)!}{(q-1)!} \sum_{j=1}^{2k-1} \frac{1}{(n-1)^j} \sum_{r=1}^{j} \frac{(-1)^{j-r} p! \log^{p-r}(n-1)}{(p-r)!} \frac{(q+2k-j-2)!}{j\,(2k-1-j)!} S_{r-1,1,j-1}$$

$$+ \frac{(2k-1)!}{(q-1)!} \sum_{j=0}^{2k-p-1} \frac{1}{(n-1)^{q+j}} \frac{(-1)^{p+j} p!(q+j-1)!}{(2k-j-1)\, j!} S_{p-1,1,2k-j-2}$$

The total expression for $\sum_{k=1}^{n-1} \frac{(\log k)^p}{(n-k)^q}$ from the Euler–Maclaurin formula is too messy to write out. As usual, cancellations will be hard at work and the result will boil down to the rhs in the lemma. The closed expression for the $D_{r,q}$ was particularly hard to find (empirically). $\square$

11

Application to the asymptotics of Stirling numbers.

Had we not known the asymptotic growth of Stirling numbers (3.2), we could easily find it by induction from the leading terms in lemma 4.2 and 6.2. Assuming the empirical result (via the asymp_k trick) that the coefficient of x^n in $(-\log(1-x))^p$ has leading behaviour $\sim p(\log n)^{p-1}/n$, we prove:

$$
\begin{aligned}
(p+1)! \sum_{n \geqslant 1} S_{p,1,n-1} \frac{x^n}{n} &= (-\log(1-x))^{p+1} = (-\log(1-x))^p \Big(\sum \frac{x^n}{n} \Big) \\
&\simeq \Big(\sum p \frac{(\log n)^{p-1}}{n} x^n \Big) \Big(\sum \frac{x^n}{n} \Big) \\
&= \sum_n x^n \frac{p}{n} \Big(\sum_{k=1}^{n-1} \frac{(\log k)^{p-1}}{k} + \sum_{k=1}^{n-1} \frac{(\log k)^{p-1}}{n-k} \Big) \\
&\simeq \sum_n x^n \frac{p}{n} \Big(\frac{(\log n)^p}{n} + (\log n)^p \Big) = (p+1) \sum_n x^n \frac{(\log n)^p}{n},
\end{aligned}
$$

hence $S_{p,1,n} \sim \frac{1}{p!}(\log n)^p$. The same inductive proof works for the next-to-leading term of (3.2). In that case, we also need the next-to-leading term of lemma 6.2. For each subsequent term that we want to prove in (3.2), we need one more term of lemma 6.2 while the leading term of lemma 4.2 is enough. One thus sees how the sequence of decreasing logarithms in (3.2) is intimately related to that of $\sum_{r=1}^p c_{p,r}(\log n)^{p-r}$ in lemma 6.2.

7   Asymptotics of sums involving $1/k^q(\log k)^p$

Lemma 7.1. *For $p \geqslant 1$ we have:*

$$
\sum_{k=2}^{n-1} \frac{1}{(\log k)^p} = \frac{1}{(p-1)!} \, \text{li}(n) - n \sum_{r=1}^{p-1} \frac{c_{p,r}}{(\log n)^r} + C_{p,0} - \frac{1}{2} \frac{1}{(\log n)^p} - \sum_{k=1}^m \Big(\sum_{r=1}^{2k-1} \frac{d_{p,r,k}}{(\log n)^{r+p}} \Big) \frac{1}{n^{2k-1}} + O(\tfrac{1}{n^{2m}}),
$$

with $c_{p,r} := \frac{(r-1)!}{(p-1)!}$ and $d_{p,r,k} := \frac{B_{2k}}{2k(2k-1)} \frac{(p-1+r)!}{(p-1)!} S_{r-1,1,2k-2}$, and $C_{p,0}$ is the constant term. The log-integral is defined by $\text{li}(z) := \int_0^z \frac{dt}{\log t}$.

Proof. This follows from the Euler–Maclaurin formula with $f(x) := \frac{1}{(\log x)^p}$ and

$$
\int f(x) = \tfrac{1}{(p-1)!} \, \text{li}(x) - x \sum_{r=1}^{p-1} \frac{(r-1)!}{(p-1)!} \frac{1}{(\log x)^r}
$$

$$
f^{(i)}(x) = (-1)^i (i-1)! \sum_{r=1}^i \frac{(p-1+r)!}{(p-1)!} \frac{S_{r-1,1,i-1}}{x^i (\log x)^{r+p}}.
$$

From these, it is also straightforward to write down the 'exact' expression for the constant $C_{p,0}$, involving a formal (infinite) sum over Bernoulli numbers. We omit it as it is not enlightening. □

Note that the second sum on the rhs is just the start of the asymptotic expression of the first term, since $\text{li}(n) \approx n \sum_{r \geqslant 1} \frac{(r-1)!}{(\log n)^r}$. So we might replace the two terms by $\frac{n}{(p-1)!} \sum_{r \geqslant p} \frac{(r-1)!}{(logn)^r}$. This is indeed what one obtains when numerically looking for the asymptotics of the lhs; the first term is $\frac{n}{(\log n)^p}$, and correctly so. Yet since this asymptotic expansion diverges for all values n, the replacement would be disastrous for numerical evaluation of the constant $C_{p,0}$.

Lemma 7.2. *For $p \geqslant 1$ we have:*

$$\sum_{k=2}^{n-1} \frac{1}{k\,(\log k)^p} = C_{p,1} - \frac{1}{(p-1)(\log n)^{p-1}} - \frac{1}{2}\frac{1}{n(\log n)^p} - \sum_{k=1}^{m}\Big(\sum_{r=0}^{2k-1}\frac{d_{p,r,k}}{(\log n)^{r+p}}\Big)\frac{1}{n^{2k}} + O(\tfrac{1}{n^{2m+1}}),$$

with $d_{p,r,k} := \frac{B_{2k}}{2k}\frac{(p-1+r)!}{(p-1)!}S_{r,1,2k-1}$, and $C_{p,1}$ is the constant term.

For $p = 1$, the second term on the rhs has to be replaced by $\log(\log n)$ (which becomes the leading term).

Proof. This follows from the Euler–Maclaurin formula with $f(x) := \frac{1}{x\,(\log x)^p}$ and

$$\int f(x) = -\frac{1}{(p-1)(\log x)^{p-1}} \qquad (p \geqslant 2)$$

$$f^{(i)}(x) = (-1)^i i! \sum_{r=0}^{i}\frac{(p-1+r)!}{(p-1)!}\frac{S_{r,1,i}}{x^{i+1}\,(\log x)^{r+p}}.$$

□

Lemma 7.3. *For $p \geqslant 1$ and $q \geqslant 2$ we have:*

$$\sum_{k=2}^{n-1}\frac{1}{k^q\,(\log k)^p} = C_{p,q} + \frac{(1-q)^{p-1}}{(p-1)!}\mathrm{Ei}((1-q)\log n) - \frac{1}{n^{q-1}}\sum_{r=1}^{p-1}\frac{c_{p,q,r}}{(\log n)^r} - \frac{1}{2}\frac{1}{n^q(\log n)^p}$$

$$- \sum_{k=1}^{m}\Big(\sum_{r=0}^{2k-1}\frac{d_{p,q,r,k}}{(\log n)^{r+p}}\Big)\frac{1}{n^{2k-1+q}} + O(\tfrac{1}{n^{2m+q}}),$$

with $c_{p,q,r} := \frac{(1-q)^{p-1-r}(r-1)!}{(p-1)!}$ and $d_{p,r,k} := \frac{B_{2k}(2k+q-2)!}{(2k)!(q-1)!}\frac{(p-1+r)!}{(p-1)!}S_{r,q,2k+q-2}$, and $C_{p,q}$ is the constant term.

The exponential integral function is defined by the principle value of the integral: $\mathrm{Ei}(x) := -\int_{-x}^{\infty}\frac{e^{-t}}{t}dt$.

Proof. This follows from the Euler–Maclaurin formula with $f(x) := \frac{1}{x^q\,(\log x)^p}$ and

$$\int f(x) = \frac{(1-q)^{p-1}}{(p-1)!}\mathrm{Ei}((1-q)\log x) - \frac{1}{x^{q-1}}\sum_{r=1}^{p-1}\frac{(r-1)!}{(p-1)!}\frac{(1-q)^{p-1-r}}{(\log x)^r}$$

$$f^{(i)}(x) = (-1)^i\frac{(i+q-1)!}{(q-1)!}\sum_{r=0}^{i}\frac{(p-1+r)!}{(p-1)!}\frac{S_{r,q,i+q-1}}{x^{i+q}\,(\log x)^{r+p}}.$$

□

Again, the third term on the rhs is just the start of the asymptotic expansion of the second term, since $\mathrm{Ei}((1-q)n) \approx \sum_{r \geqslant 1}\frac{(r-1)!}{(1-q)^r(\log n)^r}$. So we might replace both terms by the infinite sum $n^{q-1}\sum_{r \geqslant p}\frac{c_{p,q,r}}{(\log n)^r}$. But since this diverges for all n, the replacement is disastrous for numerically computing the constant $C_{p,q}$.

Note that when $p \geqslant 2$, the previous lemma makes sense also for $q = 1$, and one recovers the preceding lemma (since $(1-q)^{p-1-r}$ vanishes unless $r = p-1$).

For large p or large q, it is quite obvious that the main contribution to the sum $\sum_{k=2}^{n-1}\frac{1}{k^q\,(\log k)^p}$ comes from the term $k = 2$ and that the constants $C_{p,q}$ will converge towards $\frac{1}{2^q\,(\log 2)^p}$. Just how quick they converge can be empirically determined: asymptotically for large p or q, we have

$$C_{p,q} \sim \frac{1}{2^q\,(\log 2)^p} + e^{-ap-bq} + e^{-cp-dq} + \dots,$$

with $a = 0.09405, b = 1.0986, c = 0.3266, d = 1.386$. Of course, these values are nothing but $\log(\log 3)$, $\log 3, \log(\log 4), \log 4$, so as to obtain $\frac{1}{3^q(\log 3)^p} + \frac{1}{4^q(\log 4)^p}$! So we come back from where we started. This

comes as no surprise when $C_{p,q} = \sum_{k=2}^{\infty} \frac{1}{k^q \ (\log k)^p}$, but it is a surprise when the infinite sum does not converge, ie. when $C_{p,q}$ is not the leading term in the asymptotics, eg. when $q = 0$ and p becomes large.

$C_{p,q}$	$q = 0$	1	2	3	4
$p = 1$:	−0.24324	0.794679	0.605522	0.237996	0.106201
2:	3.10329	2.10974	0.692606	0.305808	0.143463
3:	4.96079	2.06589	0.882388	0.412914	0.199091
4:	6.00344	2.55912	1.18928	0.573295	0.28066
5:	7.46574	3.42982	1.65131	0.808652	0.399314
6:	9.92015	4.75831	2.33023	1.15106	0.571244
$2^{-q}(\log 2)^{-p}$	$q = 0$	1	2	3	4
$p = 1$:	1.4427	0.721348	0.360674	0.180337	0.0901684
2:	2.08137	1.04068	0.520342	0.260171	0.130086
3:	3.00278	1.50139	0.750695	0.375348	0.187674
4:	4.3321	2.16605	1.08302	0.541512	0.270756
5:	6.24989	3.12495	1.56247	0.781237	0.390618
6:	9.01669	4.50835	2.25417	1.12709	0.563543

Table 1: Comparison between $C_{p,q}$ and $\frac{1}{2^q(\log 2)^p}$.

We may want to add $\mathrm{li}(2) = 1.045$ to $C_{1,0}$ so as to obtain the constant $\lim_{n \to \infty} \left(\sum_{k=2}^{n-1} \frac{1}{\log k} - \int_2^n \frac{dx}{\log x} \right) = 0.80192543$. Similarly, we add $\log(\log 2) = -0.36651$ to $C_{1,1}$, so as to obtain the constant $\lim_{n \to \infty} \left(\sum_{k=2}^{n-1} \frac{1}{k(\log k)} - \int_2^n \frac{dx}{x(\log x)} \right) = 0.4281657$. Both values already occurred in [B-77], see also [F-03]. We were not able to recognize an exact form for either of these two constants (using PARI for integer linear combinations of other constants, or using Plouffe's inverter or his Maple code).

8   Asymptotics of the Taylor coefficients of $(-z/\log(1-z))^k$

We now use lemma 7.2 to generalise a result known to Pólya [P-54] about the Taylor coefficients of a certain generating function. In 1954, Pólya [P-54] noted that

$$a_n \sim -\frac{1}{n(\log n)^2} \qquad \text{for} \qquad f(z) = \frac{z}{-\log(1-z)} =: \sum a_n z^n. \tag{8.1}$$

We shall be interested in the asymptotics of the a_n when the generating function is raised to some power k (positive integer). For $k = 1$, the series begins as $1 - \frac{1}{2}x - \frac{1}{12}x - \dots$ and all coefficients are negative except a_0. The a_n for $k = 2$ are asymptotically given by the convolution of those at $k = 1$, viz. $a_n = \sum \frac{1}{i(\log i)^2 \ (n-i)(\log(n-i))^2}$. Since this sum makes only sense for i running from 2 to $n - 2$, we write

the terms $-\frac{1}{n(\log n)^2} - \frac{-1/2}{(n-1)(\log(n-1))^2} \simeq -\frac{1/2}{n(\log n)^2}$ twice separately. By symmetry, we can write:

$$a_n \approx -\frac{1}{n(\log n)^2} + 2\sum_{i=2}^{(n-2)/2} \frac{1}{i(\log i)^2} \frac{1}{(n-i)(\log(n-i))^2},$$

where in the last sum, $\log(n-i) \geqslant \log n/2$ and $\frac{1}{i(n-i)} = \frac{1/n}{i} + \frac{1/n}{n-i}$. From lemma 7.2 we know that $\sum^{n/2} \frac{1}{i(\log i)^2} = C - \frac{1}{(\log n/2)} + O(\frac{1}{(\log n/2)^2})$, wherein the constant C is figurative, since the quantities $1/(i(\log i)^2)$ only approximate the exact values of the Taylor coefficients. Further, $\sum^{n/2} \frac{1}{(n-i)(\log i)^2} \leqslant \frac{1}{n/2} \sum^{n/2} \frac{1}{(\log i)^2} = O(\frac{1}{(\log n)^2})$. Overall:

$$a_n \approx -\frac{1}{n(\log n)^2} + \frac{2C}{n(\log n)^2} - \frac{2}{n(\log n)^3} + O\Big(\frac{1}{n(\log n)^4}\Big).$$

Since the singularity of $f(z)^2$ at $z = 1$ is of higher order than that of $f(z)$, the decrease of coefficients should be stronger; hence the $\frac{1}{n(\log n)^2}$ terms have to cancel each other and so $C = 1/2$. We are left with $a_n \approx -\frac{2}{n(\log n)^3} + \dots$. One similarly obtains:

$$a_n \approx -\frac{k}{n(\log n)^{k+1}} + O\Big(\frac{1}{n(\log n)^{k+2}}\Big) \qquad \text{for} \qquad f(z) = \Big(\frac{z}{-\log(1-z)}\Big)^k. \tag{8.2}$$

A naive attempt at justifying Pólya's result (8.1) would be to use Cauchy's formula $a_n = \frac{1}{2\pi i} \oint_C \frac{f(z)\,dz}{z^{n+1}}$ and to compute the contour integral on the unit circle, $z = e^{i\theta}$. Note that $-\log(1-e^{i\theta}) = -\log(-2ie^{i\theta/2}\sin\frac{\theta}{2})$. Thus we would have (wrongly)

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} \frac{e^{-i(n-1)\theta}d\theta}{i\frac{\pi-\theta}{2} - \log(2\sin\frac{\theta}{2})} \simeq \frac{1}{2\pi} \int_0^{c/n} \frac{d\theta}{-\log\theta} \qquad \approx \frac{c/(2\pi)}{n\log n} + O\Big(\frac{1}{n(\log n)^2}\Big)$$

where we replaced $\int_0^{2\pi}$ by $\int_0^{c/n}$ since for large n, only small values of θ will contribute substantially to the integral. This approximation, however, does not yield the desired result – presumably because one cannot replace $e^{-i(n-1)\theta}$ by 1. Similarly, had we used partial integration with $f'(\theta) = \frac{e^{i\theta}\frac{1}{2}\cot\frac{\theta}{2}}{(i\frac{\pi-\theta}{2} - \log(2\sin\frac{\theta}{2}))^2}$, we would have ended up with $\frac{1}{2\pi i n} \int_0^{c/n} \frac{e^{-in\theta}d\theta}{\theta(\log\theta)^2} \approx \frac{c/(2\pi)}{n\log n}$, again with the wrong leading term. As the integral is not tractable by the Laplace method, the saddle point method or any other trick described in [dB-58], we shall see in the next subsection that the solution lies in a clever choice of the contour of integration.

The result (8.2) is not new, but was already obtained by Nörlund in 1961 using combinatorics of Bernoulli polynomials, and rederived by Flajolet and Odlyzko in 1990 by evaluating the contour integral in Cauchy's formula. For completeness, we present these two alternative and elegant paths below.

8.1 The Flajolet–Odlyzko approach

In 1990, Flajolet and Odlyzko summerised the 'transfer properties' of analytic functions, viz. the behaviour of the function at the first singularity on the convergence radius is directly reflected in the behaviour of the Taylor coefficients. One of their result is [FO-90]:

Theorem 8.3. *(Flajolet–Odlyzko, 1990) Let $f(z)$ be analytic in $|z| < 1 + \eta$ except for a singularity at $z = 1$, and let*

$$f(z) = O\Big((1-z)^\alpha(-\log(1-z))^\gamma\Big) \quad as \quad z \to 1 \quad (\alpha, \gamma \in \mathbb{R}).$$

Then the coefficients a_n in $f(z) = \sum a_n z^n$ grow like $a_n = O\Big(\frac{(\log n)^\gamma}{n^{\alpha+1}}\Big).$

Proof. (sketchy). It is comforting to see that the proof boils down to a mere application of the Cauchy formula, ie. a contour integral around the origin, viz. $a_n = \frac{1}{2\pi i} \oint_C \frac{f(z)\, dz}{z^{n+1}}$, but the contour has to be chosen cleverly – as in figure 1.
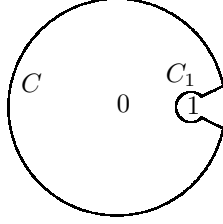

Figure 1: The contour of integration, excluding the singularity at $z = 1$.

The contour C will be a circle of radius $1 + \eta$ with a tiny roundabout around the singularity; the main contribution will come from this little near-circle C_1 (of radius $1/n$) around $z = 1$. Note that for any compact domain inside our contour C, there is a constant K such that $|f(z)| \leqslant K|(1-z)^\alpha(-\log(1-z))^\gamma|$. On the circle C_1, we have $1 - z = e^{i\theta}/n$ and the following bounds: $|f| \leqslant K(\frac{1}{n})^\alpha \sup|\log(ne^{-i\theta})|^\gamma = O\Big(\frac{(\log n)^\gamma}{n^\alpha}\Big)$, as well as $|z|^{n+1} \geqslant (1 - \frac{1}{n})^{n+1} \to 1$ and $\int_{C_1} |dz| \leqslant 2\pi/n$. Hence the main contribution to the contour integral can be estimated by: $a_n \approx \frac{1}{2\pi} \oint_{C_1} \frac{|f(z)|\, |dz|}{|z|^{n+1}} = \Big(\frac{(\log n)^\gamma}{n^{\alpha+1}}\Big)$, as we wished. $\qquad\square$

This result was readily obtained, but is treacherous when α is a non-negative integer, say 0: the Taylor coefficients of $-\log(1-z)$ decrease like $1/n$ and not like $(\log n)/n$, and those of $1/(-\log(1-z))$ decrease like $1/(n(\log n)^2)$ and not like $1/(n(\log n))$. For this case, it is useful to have a precise asymptotic development, whose derivation we sketch as follows (see [FO-90] for details). Let $f(z)$ be the function $(1-z)^\alpha(-\frac{1}{z}\log(1-z))^\gamma$. Change to the variable $z = 1 + t/n$ and expand $\log(-n/t)^\gamma = (\log n)^\gamma \sum_{i \geqslant 0} \binom{\gamma}{i}\Big(-\frac{\log(-t)}{\log n}\Big)^i$. The contour integral now contains the piece $G_i := \frac{1}{2\pi i} \int_{C_2} (-t)^\alpha(\log(-t))^i e^{-t} dt$, whose contour can be deformed to a well-known integral that simply yields $G_i = \partial_\alpha^i \frac{1}{\Gamma(-\alpha)}$. Hence the main contribution from the Cauchy formula for $f(z) = \sum a_n z^n$ is:

$$a_n \approx \frac{(\log n)^\gamma}{n^{\alpha+1}} \sum_{i \geqslant 0} \frac{(-1)^i \binom{\gamma}{i} G_i}{(\log n)^i} \qquad \text{for} \qquad f(z) = (1-z)^\alpha(-\frac{1}{z}\log(1-z))^\gamma. \qquad (8.4)$$

The first term of the sum, $i = 0$, yields $\frac{1}{\Gamma(-\alpha)}$ and thus simply drops out when α is a non-negative integer (where $\Gamma(-\alpha)$ has a pole). This explains the above treachery. For $\alpha = 0$ and $\gamma = -k$ (negative integer), we have $\binom{-k}{i} = (-1)^i \binom{k+i-1}{i}$ and $g_i := \partial_\alpha^i\big|_0 \frac{1}{\Gamma(-\alpha)} = -1, 2\gamma, -3\gamma^2 + \frac{\pi^2}{2}, \ldots (i = 1, 2, \ldots)$, and so obtain

our sought-for asymptotics:

$$a_n \approx \sum_{i \geqslant 1} \frac{\binom{k+i-1}{i} g_i}{n \, (\log n)^{i+1}} = \frac{-k}{n(\log n)^2} + \dots \qquad \text{for} \qquad f(z) = \left(\frac{z}{-\log(1-z)}\right)^k. \tag{8.5}$$

8.2 Nörlund's approach

Most surprisingly, (8.4) was arrived at 20 years earlier from quite a different angle, namely by Nörlund [N-61] who recognized the Taylor coefficients a_n of $f(z)$ as being values of generalised Bernoulli polynomials:

$$(1-z)^\alpha \left(-\frac{1}{z} \log(1-z)\right)^\gamma = \sum_{n \geqslant 0} \frac{(-z)^n}{n!} B_n^{(n+\gamma+1)}(\alpha). \tag{8.6}$$

The Bernoulli polynomials of order γ are defined by

$$\left(\frac{t}{e^t - 1}\right)^\gamma e^{\alpha t} =: \sum_{n \geqslant 0} B_n^{(\gamma)}(\alpha) \frac{t^n}{n!}$$

and coincide with the usual Bernoulli polynomials for $\alpha = 0$ (and thus yield the Bernoulli numbers for $\gamma = 1$). To arrive at (8.6), use Cauchy's formula $\frac{B_n^{(\gamma)}(\alpha)}{n!} = \frac{1}{2\pi i} \oint \frac{t^{\gamma-n-1} e^{\alpha t}}{(e^t-1)^\gamma} dt$, then substitute $t = \log(1-z)$ and shift $\gamma \to \gamma + n + 1$; you thus obtain the Cauchy formula equivalent to (8.6). At $\alpha = 1$ and $\gamma \geqslant 0$, we recover the Stirling numbers of first kind:

$$(-1)^n \, B_n^{(n+\gamma+1)}(1) = \left[\begin{matrix} n+\gamma \\ \gamma \end{matrix}\right] \Big/ \binom{n+\gamma}{\gamma} = \frac{n! \gamma!}{n+\gamma} \, S_{\gamma-1,1,n+\gamma-1}$$

The polynomials satisfy

$$B_n^{(\gamma)}(\alpha) = \int_\alpha^{\alpha+1} B_n^{(\gamma+1)}(t) \, dt \qquad \text{and} \qquad B_n^{(n+1)}(\alpha) = (\alpha-1)(\alpha-2)\cdots(\alpha-n)$$

$$= (-1)^n (n-\alpha)\cdots(1-\alpha) = (-1)^n \frac{\Gamma(n-\alpha+1)}{\Gamma(1-\alpha)}$$

Hence we can readily obtain an asymptotic expression for $\underline{\alpha = 0 \text{ and } \gamma = -1}$:

$$\frac{(-1)^n \, B_n^{(n)}(\alpha)}{n!} = \int_0^1 \frac{\Gamma(n+1-\alpha-t)}{\Gamma(1-\alpha-t)\Gamma(n+1)} \, dt$$

$$= \int_0^1 n^{-\alpha-t} \left(\frac{1}{\Gamma(1-\alpha-t)} + O(\tfrac{1}{n})\right)$$

$$= n^{-\alpha} \left[\frac{1}{(\log n)\Gamma(1-\alpha)} - \int_0^1 \frac{e^{-t \log n}}{-\log n} \, \partial_t \frac{1}{\Gamma(1-\alpha-t)} dt + O\big(\tfrac{1}{n \log n}\big)\right]$$

where we used Stirling's approximation $n! \sim e^{n \log n - n + \frac{1}{2} \log(2\pi n)}$ in the second step and partial integration in the third step. Further partial integrations yield

$$\frac{(-1)^n \, B_n^{(n)}(\alpha) \, n^\alpha}{n!} = \sum_{i=0}^{r-1} \frac{1}{(\log n)^{i+1}} \, \partial_\alpha^i \frac{1}{\Gamma(1-\alpha)} + O\big(\tfrac{1}{(\log n)^{r+1}}\big)$$

where the derivative term evaluated at $\alpha = 1$ is: $\partial_\alpha^i \big|_1 \frac{1}{\Gamma(1-\alpha)} = \partial_\alpha^i \big|_0 \frac{1}{\Gamma(-\alpha)} =: g_i$, with $g_i = 0, -1, 2\gamma, -3\gamma^2 + \frac{\pi^2}{2}, \dots$ for $i = 0, 1, \dots$. Overall:

$$a_n = \frac{(-1)^n \, B_n^{(n)}(1)}{n!} \approx \sum_{i \geqslant 1} \frac{g_i}{n(\log n)^{i+1}} \qquad \text{for} \qquad f(z) = \frac{z}{-\log(1-z)}.$$

From here, it is straightforward (via induction) to deduce the general case $\gamma = -k$ (negative integer):

$$a_n = \frac{(-1)^n \ B_n^{(n-k+1)}(1)}{n!} \approx \sum_{i \geqslant 1} \frac{\binom{k+i-1}{i} g_i}{n(\log n)^{i+1}} = \frac{-k}{n(\log n)^2} + \dots \qquad \text{for} \qquad f(z) = \left(\frac{z}{-\log(1-z)}\right)^k$$

in full agreement with (8.5)

9 Asymptotics of the incomplete Gamma function

This sections examines whether the constant $C_{1,1}$ met in section 7 also occurs in the constant term of the the function $\sum_{n=2}^{\infty} \frac{1}{(n \log n)^s}$. The answer is yes, as the general theory shows, but γ has to be subtracted to obtain the full constant term. The resulting expansion is presented in (9.2), and on the way we shall derive the following intermediate result about the asymptotics of the incomplete gamma function (a is an arbitrary constant):

$$\Gamma(-s, as) := \int_{as}^{\infty} t^{-s-1} e^{-t} dt = -\log(as) - \gamma + s[\tfrac{1}{2}(\log(as))^2 + a - c_1] + O(s^2 \log^3(as)) \qquad \text{as } \ s \to 0.$$

9.1 Preliminaries

Recall the coincidence in the constant terms of the following asymptotic expansions:

$$\zeta(s) = \sum_{k \geqslant 1} \frac{1}{k^s} \approx \frac{1}{s-1} + \gamma - \gamma_1(s-1) + \dots \qquad (s \to 1)$$

$$\sum_{k=1}^{n-1} \frac{1}{k} \approx \log n + \gamma - \frac{1}{2n} + \dots \qquad (n \to \infty)$$

Landau confirmed this coincidence for a broader class of Dirichlet series: suppose $\sum_{n \leqslant x} h(n) \sim \alpha x + \dots$ (among other constraints on $h(n)$), then:

$$\sum_{n=1}^{\infty} \frac{h(n)}{n^s} \approx \frac{\alpha}{s-1} + \beta + \dots \qquad (s \to 1^+)$$

for some constant β, and

$$\sum_{n \leqslant x} \frac{h(n)}{n} \approx \alpha \log x + \beta + \dots \qquad (x \to \infty).$$

We shall be concerned with a weaker generalisation. First recall the discrete partial integration formula for some continuous function ϕ and some sequence a_n with primitive $A(x) := \sum_{n \leqslant x} a_n$:

$$\sum_{n=a+1}^{b} a_n \phi(n) = A(x)\phi(x) \Big|_a^b - \int_a^b A(x)\phi'(x) dx.$$

When $a, b \in \mathbb{Z}$ and $a_n = 1$ with $A(x) = \lfloor x \rfloor$, the formula reduces to

$$\sum_{n=a}^{b} \phi(n) = x\phi(x) \Big|_a^b - \int_a^b \lfloor x \rfloor \phi'(x) dx + \phi(a)$$

$$= \int_a^b \phi + \int_a^b (x - \lfloor x \rfloor)\phi' + \phi(a).$$

If $\phi_s(x)$ is a suitable function depending on a parameter s, like $\phi_s(x) = \frac{1}{x^s}$, the derivative in the second integrand will ensure that we may exchange the limits $b \to \infty$ and $s \to 1$ (since $x - \lfloor x \rfloor$ is bounded). In other words, the first integral contains the singularity as $s \to 1$, while the second integral yields merely a constant. Denote by ϕ_1 the function ϕ_s obtained after taking the limit $s \to 1$; we then perform the partial integration backwards:

$$\int_a^b (x - \lfloor x \rfloor)\phi_1' = \sum_{k=a}^{b-1} \int_k^{k+1} (x-k)\phi_1' = \sum_{k=a}^{b-1} \left(\phi_1(k+1) - \int_k^{k+1} \phi_1 \right) = \sum_{k=a+1}^{b} \phi_1(k) - \int_a^b \phi_1.$$

Having previously taken the limit $b \to \infty$, we obtain our desired generalisation:

$$\lim_{s \to 1} \left(\sum_{n=a}^{\infty} \phi_s(n) - \int_a^{\infty} \phi_s \right) = \lim_{b \to \infty} \left(\sum_{k=a}^{b} \phi_1(k) - \int_a^b \phi_1 \right).$$

For instance, for $\phi_s(x) = \frac{1}{x^s}$ and $a = 1$, we have:

$$\lim_{s \to 1} \left(\zeta(s) - \frac{1}{s-1} \right) = \lim_{b \to \infty} \left(H_b - \log b \right) = \gamma.$$

For $\phi(x) = \frac{1}{(x \log x)^s}$ and $a = 2$, we have by lemma 7.2:

$$\lim_{s \to 1} \left(\sum_{n=2}^{\infty} \frac{1}{(n \log n)^s} - \int_2^{\infty} \frac{dx}{(x \log x)^s} \right) = \lim_{b \to \infty} \left(\sum_{n=2}^{b} \frac{1}{n \log n} - \log(\log b) + \log(\log 2) \right) = C_{1,1} + \log(\log 2).$$

$$(9.1)$$

9.2   Gamma function asymptotics

In order to find the constant term in the asymptotics of the function $\sum_{n=2}^{\infty} \frac{1}{(n \log n)^s}$, we still need to expand the corresponding integral up to the constant term. This will include finding its singularity at $s = 1$. Note first that

$$\int_2^{\infty} \frac{dx}{(x \log x)^s} = (s-1)^{s-1} \ \Gamma(1-s, \ (s-1)\log 2) = (s-1)^{s-1} \int_{(s-1)\log 2}^{\infty} t^{-s} e^{-t} dt.$$

The incomplete Gamma function is defined by $\Gamma(z, s) := \int_s^{\infty} t^{z-1} e^{-t} dt$. Hence $\frac{d}{ds}\Gamma = \Gamma_z \frac{dz}{ds} + \Gamma_s$. To simplify matters, we shall first study the behaviour of $\Gamma(-s, s)$ as $s \to 0$. Note that $\Gamma(0, s) \sim -\log s - \gamma + \ldots$ and $\Gamma(-s, 0) \sim -\frac{1}{s} - \gamma + \ldots$, so that the simultaneous limit will behave like the weaker of both, ie $\lim_{s \to 0} \Gamma(-s, s) \sim -\log s + \ldots$. Equipped with this intuition, we proceed by expanding $\partial_s \Gamma(-s, s)$ (around $s = 0$) and then integrating the expanded result. Now with $z(s) = -s$ we have

$$\frac{d}{ds}\Gamma(-s, s) = \left[\frac{\partial \Gamma}{\partial z} \frac{dz}{ds} + \frac{\partial \Gamma}{\partial s} \right]_{z=-s} = -e^{-s} s^{-s-1} - \int_s^{\infty} t^{-s-1} e^{-t} (\log t) dt.$$

The first part is expanded as $-e^{-s} s^{-s-1} = -\frac{1}{s} e^{-s(1+\log s)} = -\frac{1}{s} + (\log s + 1) + \ldots$ and gives us – upon integration – the required $(-\log s)$ term, so that the second part can contain at most log-singularities. Differentiating the latter gives us $e^{-s} s^{-s-1} \log s + \int_s^{\infty} t^{-s-1} e^{-t} (\log t)^2 dt$, which behaves as $(\log s)/s + \ldots$,

so that the original integral behaves as $\frac{1}{2}(\log s)^2 +$ const $+ \ldots$. In general, $\int_s^\infty t^{-s-1}e^{-t}(\log t)^i dt$ will

behave as $-\frac{1}{i+1}(\log s)^i +$ const $+ \ldots$, and by bootstrapping we obtain:

$$\int_s^\infty t^{-s-1}e^{-t}dt = -(\log s) + c_0 + s[\tfrac{1}{2}(\log s)^2 + 1 - c_1] + \ldots$$

$$\int_s^\infty t^{-s-1}e^{-t}(\log t)dt = -\tfrac{1}{2}(\log s)^2 + c_1 + s[\tfrac{1}{3}(\log s)^3 + (\log s) - 1 - c_2] + \ldots$$

$$\vdots$$

$$\int_s^\infty t^{-s-1}e^{-t}(\log t)^i dt = -\tfrac{1}{i+1}(\log s)^{i+1} + c_i + s\left[\tfrac{1}{i+2}(\log s)^{i+2} + \sum_{r=0}^i \frac{(-1)^{r+i}i!}{r!}(\log s)^r - c_{i+1}\right] + \ldots$$

In this way, we can start with the n-th line at order $O(s)$ and recursively determine the expansion of the

first line up to $O(s^n)$ in terms of the constants of integration $c_0, \ldots, c_n$. The latter can be empirically

determined: $c_0 = -\gamma$, $c_1 = 0.98905$, $c_2 = -1.81497$, $c_3 = 5.89038$, $c_4 = -23.568$, etc. We have computed

the first 300 of them and it seems that their asymptotics are $c_i = (-1)^{i+1}(i! - e^{0.8\, i \log i} + \ldots)$. It would

be interesting to know more about these constants. In particular, we obtain our desired expansion:

$$\Gamma(-s, s) = -(\log s) - \gamma + s[\tfrac{1}{2}(\log s)^2 + 1 - c_1] + s^2\left[-\tfrac{1}{6}(\log s)^3 - (\log s) + \tfrac{3}{4} + \tfrac{c_2}{2}\right] + \ldots \qquad (s \to 0)$$

Next, study $\Gamma(-s, as)$ for some constant a. Now $\frac{d}{ds}\Gamma = \Gamma_z(-1) + \Gamma_s a$. Bootstrapping yields now:

$$\int_{as}^\infty t^{-s-1}e^{-t}(\log t)^i dt = -\tfrac{1}{i+1}(\log s)^{i+1} + c_i + s\left[\tfrac{1}{i+2}(\log s)^{i+2} + a\sum_{r=0}^i \frac{(-1)^{r+i}i!}{r!}(\log s)^r - c_{i+1}\right] + \ldots,$$

with the constants c_i taking the same values as before. In particular,

$$\Gamma(-s, as) = -\log(as) - \gamma + s[\tfrac{1}{2}(\log(as))^2 + a - c_1] + s^2\left[-\tfrac{1}{6}(\log(as))^3 - a\log(as) + \tfrac{c_2}{2} - \tfrac{a^2}{4} + a\right] + \ldots \qquad (s \to 0)$$

Thus we can answer the question above:

$$\int_2^\infty \frac{dx}{(x\log x)^s} = \left[1 + (s-1)\log(s-1) + \ldots\right]\left[-\log((s-1)\log 2) - \gamma + (s-1)[\tfrac{1}{2}\log^2((s-1)\log 2) + \log 2 - c_1] + \ldots\right]$$

$$= -\log(s-1) - (\gamma + \log\log 2) + (s-1)\left[-\tfrac{1}{2}\log^2(s-1) + (\log 2 - c_1 - \gamma)\log(s-1) + \right.$$

$$\left. + \log 2 - c_1\right] + O((s-1)^2\log^3(s-1))$$

Recalling (9.1), we deduce the constant term in the asymptotic development of the original function:

$$\sum_{n=2}^\infty \frac{1}{(n\log n)^s} \approx -\log(s-1) + C_{1,1} - \gamma + O\big((s-1)\log^2(s-1)\big) \qquad (s \to 1) \qquad (9.2)$$

where $C_{1,1} = 0.794679\ldots$ was given in table 1.

10 A representation of polylogs and of Nielsen integrals

In this section we present a representation of polylogs in terms of Nielsen integrals which we have come

across while embarking onto the proofs in section 6. Conversely, in (10.9) and (10.10) we give repre-

sentations of Nielsen integrals involving Bernoulli numbers, which boil down to mysterious identities

for Bernoulli numbers and harmonic numbers (conjecture 10.11). We only treat the cases $\mathfrak{S}_{1,1}(x)$ and $\mathfrak{S}_{1,2}(x)$, but are convinced that similar formulae hold for all $\mathfrak{S}_{1,p}(x)$.

Lemma 10.1.

$$\mathrm{Li}_2(1-x) = \zeta(2) + (\log x)\sum_1 \frac{x^n}{n} - \sum_1 \frac{x^n}{n^2} \tag{10.2}$$

$$\mathrm{Li}_3(1-x) = \zeta(3) - \zeta(2)\sum_1 \frac{x^n}{n} - (\log x)\sum_1 \frac{H_{n-1}}{n}x^n + \sum_1 \left(\frac{H_{n-1}^{(2)}}{n} + \frac{H_{n-1}}{n^2}\right)x^n \tag{10.3}$$

$$\mathrm{Li}_4(1-x) = \zeta(4) - \zeta(3)\sum_1 \frac{x^n}{n} + \zeta(2)\sum_1 \frac{H_{n-1}}{n}x^n + (\log x)\sum_1 \frac{\sum_{i=1}^{n-1}\frac{H_{i-1}}{i}}{n}x^n -$$

$$- \sum_1 \left(\frac{\sum_{i=1}^{n-1}\left(\frac{H_{i-1}^{(2)}}{i} + \frac{H_{i-1}}{i^2}\right)}{n} + \frac{\sum_{i=1}^{n-1}\frac{H_{i-1}}{i}}{n^2}\right)x^n \tag{10.4}$$

$$\mathrm{Li}_j(1-x) = \zeta(j) - \zeta(j-1)\sum_1 \frac{S_{0,1,n-1}}{n}x^n + \zeta(j-2)\sum_1 \frac{S_{1,1,n-1}}{n}x^n - \cdots + (-1)^j\zeta(2)\sum_1 \frac{S_{j-3,1,n-1}}{n}x^n$$

$$+ (-1)^j(\log x)\sum_1 \frac{S_{j-2,1,n-1}}{n}x^n - (-1)^j\sum_1 \left(\frac{T_{j-2,n-1}}{n} + \frac{S_{j-2,1,n-1}}{n^2}\right)x^n \tag{10.5}$$

with $T_{j-2,n-1} := \sum \frac{1}{i_1 \cdots i_{j-3}k^2}$ (sum over all $1 \leqslant i_1 < \cdots < i_{j-3} \leqslant n-1$ and $1 \leqslant k \leqslant n-1$, $k \neq i_1, \ldots, i_{j-3}$) satisfying the following recursion: $T_{j-2,n-1} = \sum_{i=1}^{n-1}\frac{T_{j-3,i-1}}{i} + \frac{S_{j-3,1,i-1}}{i^2}$. The last sum of (10.5) can also be written as $-\sum_{r=0}^{j-2}\mathfrak{S}_{1,j-r-1}(x)\frac{\log^r(1-x)}{r!}$ with $\mathfrak{S}_{1,p}(x) := \sum_{n\geqslant 1}\frac{S_{p-1,1,n-1}}{n^2}x^n$, that is[2] $x\partial_x \mathfrak{S}_{1,p}(x) = \frac{(-\log(1-x))^p}{p!}$ for $p \geqslant 1$. Thus the above can be rewritten as $(j \geqslant 2)$

$$\mathrm{Li}_j(1-x) = \sum_{r=0}^{j-1}\left(\zeta(j-r) - \mathfrak{S}_{1,j-r-1}(x)\right)\frac{\log^r(1-x)}{r!} \tag{10.6}$$

wherein the term with $\zeta(1)$ should be dropped.

Proof. Show the recursion $\frac{d}{d\log(1-x)}\mathrm{Li}_j(1-x) = \mathrm{Li}_{j-1}(1-x)$ using the fact that $\sum_{r=0}^{j-1}(\partial_x\mathfrak{S}_{1,j-r-1}(x))\frac{\log^r(1-x)}{r!} = \frac{\log^{j-1}(1-x)}{x}\sum_{r=0}^{j-1}\frac{(-1)^{j-1-r}}{(j-1-r)!r!} = 0$ (binomial formula for $(1-1)^{j-1}$). Note that $\frac{\log^r(1-x)}{r!}$ could be replaced by $\frac{(-\mathrm{Li}_1(x))^r}{r!}$ or by $(-1)^r\,\mathrm{Li}_{1^r}(x)$, where the generalised polylog is defined by

$\mathrm{Li}_{s_1,\ldots,s_k}(x) := \displaystyle\sum_{n_1 > \cdots > n_k > 0}\frac{x^{n_1}}{n_1^{s_1}\ldots n_k^{s_k}}$. Thus the formula could read:

$$\mathrm{Li}_j(1-x) = \sum_{r=0}^{j-1}\left(\mathrm{Li}_{j-r}(1) - \mathrm{Li}_{2,1^{j-r-2}}(x)\right)(-1)^r\,\mathrm{Li}_{1^r}(x),$$

wherein the term with $\mathrm{Li}_1(1)$ should be dropped.

$\square$

The $\mathfrak{S}_{1,p}$ are special cases of so-called *Nielsen integrals* (for $k \geqslant 1$):

$$\mathfrak{S}_{k,p}(x) := \frac{(-1)^{k+p-1}}{(k-1)!p!}\int_0^1 \frac{dy}{y}\log^{k-1}(y)\log^p(1-xy) = \sum_{n\geqslant 1}\frac{S_{p-1,1,n-1}}{n^{k+1}}x^n = \mathrm{Li}_{k+1,1^{p-1}}(x),$$

---

[2] We have used $(-\log(1-x))^p = p!\sum_{n\geqslant 0}\left[\begin{smallmatrix}n\\p\end{smallmatrix}\right]\frac{x^n}{n!} = p!\sum_{n\geqslant 0}\frac{S_{p-1,1,n-1}}{n}x^n$ which is proved by expanding: lhs $= \partial_r^p\big|_0(1-x)^{-r} = \ldots$ (notation and convention from [GKP-89])

so that $\mathfrak{S}_{k-1,1}(x) = \mathrm{Li}_k(x)$ and $x\partial_x\, \mathfrak{S}_{k,p}(x) = \mathfrak{S}_{k-1,p}(x)$. Also: $\mathfrak{S}_{1,1}(x) = \mathrm{Li}_2(x)$, $\mathfrak{S}_{1,0}(x) = \log x$.

As a corollary, equate the last term of (10.4) with the corresponding quantity in (10.6) and find: $\frac{1}{n}\sum_{i=1}^{n-1}\left(\frac{H_{i-1}^{(2)}}{i} + \frac{H_{i-1}}{i^2}\right) = \sum_{i=1}^{n-1}\left(\frac{H_{i-1}}{i(n-i)^2} - \frac{H_{i-1}}{i^2(n-i)}\right)$; or, using partial fractions:

$$\sum_{i=1}^{n-1}\frac{H_{i-1}}{(n-i)^2} = \sum_{i=1}^{n-1}\left(\frac{H_{i-1}^{(2)}}{i} + 2\frac{H_{i-1}}{i^2}\right),$$

which can easily be generalised:

Lemma 10.7. *For $p \geqslant 1$:*

$$\sum_{i=1}^{n-1}\frac{H_{i-1}}{(n-i)^p} = \sum_{i=1}^{n-1}\left(\sum_{r=1}^{p-1}\frac{H_{i-1}^{(p-r+1)}}{i^r} + 2\frac{H_{i-1}}{i^p}\right).$$

Proof. lhs $= \sum_{i=1}^{n-1}\frac{H_{n-i-1}}{i^p} = \sum_{i=1}^{n-1}\sum_{j=1}^{n-i-1}\frac{1}{i^p j} = \sum_{j=1}^{n-1}\sum_{i=1}^{j-1}\frac{1}{i^p(j-i)} =$ rhs, using the partial fractions $\frac{1}{i^p(j-i)} = \sum_{r=1}^{p}\frac{1}{i^r j^{p-r+1}} + \frac{1}{(j-i)j^p}$. $\qquad\square$

Lemma 10.8. *With $b_i := \sum_{r=1}^{i}\frac{(-1)^r B_r}{r}$, we have for $|x| < 1$:*

$$\mathfrak{S}_{1,1}(x) = \mathrm{Li}_2(x) = \sum_{i\geqslant 1}\left(\frac{(-1)^i B_i}{i^2}x^i - \frac{b_i}{i}\left(\frac{x}{x-1}\right)^i\right) \tag{10.9}$$

$$\mathfrak{S}_{1,2}(x) = \sum_{n\geqslant 1}\frac{H_{n-1}}{n^2}x^n = \sum_{i\geqslant 1}\left(\frac{(-1)^i B_i H_{i-1}}{i^2}x^i - \frac{b_i}{i}[H_{i-1} + \mathrm{Li}_1(x)]\left(\frac{x}{x-1}\right)^i\right) \tag{10.10}$$

Proof. The first equation is equivalent to an identity for Bernoulli numbers:

$$\sum_{r=1}^{n-1}\frac{(-1)^r B_r}{r}\sum_{l=r}^{n}\frac{(-1)^l}{l}\binom{n-1}{n-l} = -\frac{1}{n^2} \qquad (n \geqslant 2)$$

in which the second sum equals $\frac{1}{n}\sum_{l=r}^{n}(-1)^l\binom{n}{l} = -\frac{1}{n}\sum_{l=0}^{r-1}(-1)^l\binom{n}{l} = -\frac{(-1)^r}{n}\binom{n-1}{r-1} = -\frac{(-1)^r r}{n^2}\binom{n}{r}$. Thus the equation boils down to the well-known identity for Bernoulli numbers: $\sum_{r=0}^{n}\binom{n}{r}B_r = B_n$ or mnemotechnically: $(B+1)^n = B_n$ (upon replacing B^k by B_k).

The second equation is equivalent to

$$-\sum_{r=1}^{p-1}\frac{(-1)^r B_r}{r}\sum_{l=r}^{p}\frac{(-1)^l}{l}\binom{p-1}{p-l}H_{l-1} - \sum_{n=1}^{p-1}\left(\sum_{r=1}^{n}\frac{(-1)^r B_r}{r}\sum_{l=r}^{n}\frac{(-1)^l}{l}\binom{n-1}{n-l}\right)\frac{1}{p-n} = \frac{H_{p-1}}{p^2}$$

or

$$-\sum_{r=1}^{p-1}\frac{(-1)^r B_r}{r}\sum_{l=r}^{p}\frac{(-1)^l}{l}\binom{p-1}{p-l}H_{l-1} - \sum_{n=1}^{p-1}\frac{(-1)^n B_n}{n^2(p-n)} + \frac{H_{p-1}^{(2)}}{p} + 2\frac{H_{p-1}}{p^2} = \frac{H_{p-1}}{p^2}$$

Note also that

$$\sum_{l=1}^{p+1}(-1)^l\binom{p+1}{l}H_{l-1} = -\sum_{l=0}^{p}\frac{(-1)^l}{l}\binom{p}{l} = H_p$$

where the second equality follows by induction, while the first comes from

$$\text{lhs} = (-1)^{p-1}\sum_{l=0}^{p}(-1)^{p-l}\binom{p+1}{p-l}H_l = (-1)^{p-1}\left[(1-x)^{p+1}\frac{-\log(1-x)}{1-x}\right]_{x^p} = (-1)^{p-1}\sum_{l=0}^{p}\frac{(-1)^{p-l}}{l}\binom{p}{p-l}.$$

Hence the second equality is equivalent to the following conjecture, which has resisted the author's best efforts. $\qquad\square$

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Conjecture 10.11. *For p a positive integer:*

$$\sum_{r=1}^{p-1} \frac{(-1)^r B_r}{r} \left(\sum_{l=r}^{p} (-1)^l \binom{p}{l} H_{l-1} + \frac{1}{r} + \frac{1}{p-r} \right) = H_{p-1}^{(2)} + \frac{1}{p} H_{p-1}.$$

Conclusion

Though an application of the Euler–Maclaurin formula is nothing distinguished, it turns out that its use for the four sums of sections 4,5,6,7 resp. brings along a wealth of by-products about Stirling numbers, their relation to harmonic numbers, their asymptotics, about mathematical constants and their representation as formal (diverging) sums over rational (Bernoulli) numbers, about more general asymptotics of complex functions (incl. incomplete gamma functions), as well as algebraic manipulations on polylogs and Nielsen integrals. All this research was only possible because we used the asymp_k trick and numerical mathematics.

Extensions of this paper would be doing the same for other sums containing logarithms, foremost $\sum k^q/(\log k)^p$, $\sum (n-k)^q (\log k)^p$, but we do not expect any new property. Perhaps only more unknown mathematical constants would come to light. Otherwise, the constants $C_{p,q}$ of section 7 still await an exact form. Further, one could attempt to prove conjecture 10.11 or write down the similar (and more complex) identities that one obtains when carefully going through the proof of lemma 6.2. Perhaps even more bizarre identities would show up by carefully analyzing what happens in the proofs of lemmas 6.3 and 6.4.

Acknowledgments

A   The asymp$_k$ trick

Assume we are given numerically the first hundreds of terms of a converging sequence (s_n), $(n \in \mathbb{N})$, and that its asymptotic expansion goes in inverse powers of n, ie. $s := c_0 + \frac{c_1}{n} + \frac{c_2}{n^2} + \dots$.

Goal: determine the coefficient c_0.

Trick (by Don Zagier): apply the operator $\frac{1}{k!} \partial^k n^k$ on s ($k \in \mathbb{N}$) to find

$$c_0 + (-1)^k \frac{c_{k+1}}{n^{k+1}} + \dots + (-1)^{k+l} \binom{k+l-1}{l-1} \frac{c_{k+l}}{n^{k+l}} + \dots$$

Hence this gives k more digits of precision for c_0, as long as k is not too big (ie. the binomials not too big). Call this operation $\underline{\text{asymp}_k}$. In practice, the operator ∂ is the difference operator $\Delta s := s_{n+1} - s_n$.

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To determine c_1, subtract c_0, multiply by n and apply asymp_k or: differentiate (ie. take successive differences) and multiply by $-n^2$.

The crucial point in the success of this trick is that the errors generated by the difference operator on a monomial are themselves monomials of lower powers: $\Delta \frac{1}{n^j} = \frac{1}{(n+1)^j} - \frac{1}{n^j} = \frac{-j}{n^{j+1}} + \frac{j(j+1)/2}{n^{j+2}} + \cdots$. These will be swept away at the next applications of Δ. The same would not be true if the operator acted on terms like $(\log n)^j$.

NB: we can see whether the k decimals are correct by checking the convergence of the series: if we have 400 terms, say, write every 80th term in a column (ie. 5 terms in total) and see how quickly the digits agree.

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