Euler-Maclaurin, harmonic sums and Stirling's formula

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Two rather accurate approximations

We consider two problems of approximation. First, consider the harmonic sum

$$H_n = \sum_{r=1}^{n} \frac{1}{r}.$$

Without computers, numerical evaluation of, say, H_{100} by direct addition would be a very tedious calculation, and even with computers it would be a very inefficient method.

With the 'lateral thinking' typical of our subject, we can do much better. Discrete sums can be approximated by corresponding integrals, which we often know how to evaluate exactly. In this case, the corresponding integral is $\int_1^n \frac{1}{x}\,dx = \ln n$. As the reader will be well aware, $H_n - \ln n$ converges to Euler's constant γ. We recall briefly the standard way to prove this. Since $\int_n^{n+1} \frac{1}{x}\,dx = \ln(n+1) - \ln n$ and $\frac{1}{n+1} \leqslant x \leqslant \frac{1}{n}$ for $n \leqslant x \leqslant n+1$, we have

$$\frac{1}{n+1} \leqslant \ln(n+1) - \ln n \leqslant \frac{1}{n}.$$

It follows that $H_n - \ln n$ is decreasing, while $H_{n-1} - \ln n$ is increasing, so both converge to a limit (which we call γ). Also, $H_n - \ln n \geqslant \gamma$ and $H_{n-1} - \ln n \leqslant \gamma$, hence we have

$$\ln n + \gamma \leqslant H_n \leqslant \ln n + \gamma + \frac{1}{n}.$$

This can be viewed as a pair of bounds for H_n, regarding γ as known: for H_{100}, the bounds (to five d.p., rounded down and up respectively) are 5.18238 and 5.19239. Alternatively, rewritten suitably, it can be viewed as a pair of bounds for γ, regarding H_n as known (for this purpose, one would wish to choose n fairly small). With $n = 10$, the bounds are 0.52638 and 0.62639: hardly impressive!

Using the convexity of $1/x$, one can improve the approximation to

$$\ln n + \gamma + \frac{1}{2n+1} \leqslant H_n \leqslant \ln n + \gamma + \frac{1}{2n}.$$

(We will not spell out the details here.) The difference between the upper and lower bounds is now $1/[2n(2n+1)]$. The resulting bounds for H_{100} are 5.187361 and 5.187386, and those implied for γ, again with $n = 10$, are 0.57638 and 0.57877.

In this article we will show how to establish, without excessive effort, the following dramatically more accurate approximation:

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Theorem 1:

$$H_n = \ln n + \gamma + \frac{1}{2n} - \frac{1}{12n^2} + r_n, \tag{1}$$

where

$$0 \leqslant r_n \leqslant \frac{1}{120n^4}. \tag{2}$$

This gives $H_{100} = 5.18737752$ to eight d.p. (note that the term r_n is less than 10^{-10}), and the bounds for γ, with $n = 10$, are 0.57721566 (which actually agrees with the true value to eight d.p.) and 0.57721650.

Our second approximation is Stirling's formula. In its integer form, this states

$$n! \sim Cn^{n+\frac{1}{2}}e^{-n} \text{ as } n \to \infty,$$

where $C = \sqrt{2\pi}$ and the notation $f(n) \sim g(n)$ means that $f(n)/g(n) \to 1$. For 10! (actual value 3,628,800) the approximation is 3,598,696. Restated in logarithmic form, the statement is equivalent to

$$\ln n! = \left(n + \tfrac{1}{2}\right) \ln n - n + c + Q_n,$$

where $c = \frac{1}{2} \ln(2\pi)$ and $Q_n \to 0$ as $n \to \infty$. We will establish the following much more accurate version:

Theorem 2:

$$\ln n! = \left(n + \tfrac{1}{2}\right) \ln n - n + c + \frac{1}{12n} - q_n, \tag{3}$$

where

$$0 \leqslant q_n \leqslant \frac{1}{360n^3}. \tag{4}$$

For 10!, these bounds, to the nearest integer, are 3,628,800 itself and 3,628,810.

We will prove both theorems (in the case of Theorem 1, a more general result) by a truncated version of the powerful technique known as Euler-Maclaurin summation. This process has other applications; we will describe one, the estimation of the sum of a convergent series.

Euler-Maclaurin summation

The following is an attempt at a motivated exposition of Euler-Maclaurin summation, taking advantage of the fact that the early stages (which are all we need for Theorems 1 and 2) can easily be performed without the general theory of Bernoulli polynomials. Readers already familiar with the process could move on to Lemma 1 below, where our account begins to diverge from the usual ones.

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Consider any differentiable function f on $[0, 1]$. Let

$$J(f) = \int_0^1 f(x)\,dx.$$

We compare $J(f)$ with its estimate by the trapezium rule:

$$T(f) = \tfrac{1}{2}f(0) + \tfrac{1}{2}f(1).$$

The aim is to give an accurate estimation of the difference $T(f) - J(f)$. There is a simple integral expression for this difference:

Proposition 1:

$$T(f) - J(f) = \int_0^1 \left(x - \tfrac{1}{2}\right) f'(x)\,dx. \tag{5}$$

Proof: Integrating by parts, we obtain

$$\begin{aligned}\int_0^1 \left(x - \tfrac{1}{2}\right) f'(x)\,dx &= \left[\left(x - \tfrac{1}{2}\right) f(x)\right]_0^1 - \int_0^1 f(x)\,dx \\ &= \tfrac{1}{2}f(1) + \tfrac{1}{2}f(0) - J(f).\end{aligned}$$

To translate (5) to the interval $[r, r + 1]$, we just apply it to $f(x + r)$. Write $J_r(f) = \int_r^{r+1} f(x)\,dx$ and

$$T_r(f) = \tfrac{1}{2}f(r) + \tfrac{1}{2}f(r + 1).$$

We obtain

$$T_r(f) - J_r(f) = \int_r^{r+1} \left(x - r - \tfrac{1}{2}\right) f'(x)\,dx. \tag{6}$$

Note that the r occurring in this integral is the same as $[x]$, the integer part of x. With this observation, we can combine (6) over successive intervals, as follows. Write

$$I_n(f) = \int_1^n f(x)\,dx,$$

so that $I_n(f) = \sum_{r=1}^{n-1} J_r(f)$. Further, write

$$S_n(f) = \sum_{r=1}^{n} f(r),$$

also

$$S_n^*(f) = \sum_{r=1}^{n-1} T_r(f) = \tfrac{1}{2}f(1) + \sum_{r=2}^{n-1} f(r) + \tfrac{1}{2}f(n) \qquad (n \geqslant 2)$$

and $S_1^*(f) = 0$, so that $S_n(f) = S_n^*(f) + \frac{1}{2}f(1) + \frac{1}{2}f(n)$. Adding (6) for $1 \leqslant r \leqslant n - 1$, we obtain

$$S_n^*(f) - I_n(f) = \int_1^n \left(x - [x] - \tfrac{1}{2}\right) f'(x)\,dx. \tag{7}$$

This is the most elementary version of the Euler-Maclaurin sum formula, and it has its uses, for example for extending the definition of the Riemann

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zeta function $\zeta(s)$ beyond the region $\mathrm{Re}\, s > 1$ of the complex plane where the series $\sum_{n=1}^{\infty} n^{-s}$ converges.

However, we can improve greatly on (7) by working on the right-hand side. We confine attention to real-valued functions. We will describe the whole process for the interval [0, 1], and only subsequently translate to other intervals as above.

Consider the integral in (5), split into two integrals on $\left[0, \frac{1}{2}\right]$ and $\left[\frac{1}{2}, 1\right]$. If $f'(x)$ is of one sign and does not vary too much, the the two contributions will be of opposite sign and close in magnitude, resulting in a good deal of cancellation. An estimate capturing this cancellation is found by integrating by parts the other way round, as follows:

Proposition 2:

$$T(f) - J(f) = \tfrac{1}{2}\int_0^1 \left(x - x^2\right) f''(x)\, dx. \tag{8}$$

Hence if $m \leqslant f''(x) \leqslant M$ on [0, 1], then

$$\tfrac{1}{12} m \leqslant T(f) - J(f) \leqslant \tfrac{1}{12} M. \tag{9}$$

Proof: Integrating by parts in (5), we have

$$T(f) - J(f) = \left[\tfrac{1}{2}\left(x^2 - x\right) f'(x)\right]_0^1 - \tfrac{1}{2}\int_0^1 \left(x^2 - x\right) f''(x)\, dx$$

$$= \tfrac{1}{2}\int_0^1 \left(x - x^2\right) f''(x)\, dx,$$

which is (8). Statement (9) follows, because $x - x^2 \geqslant 0$ on [0, 1] and $\int_0^1 \left(x - x^2\right) dx = \frac{1}{6}$.

In particular, if $f''(x) \geqslant 0$ on [0, 1] (so that $f(x)$ is convex), then $T(f) \geqslant J(f)$. Statement (9) is already a powerful pair of inequalities. Some applications were described in [1]. In particular, for the harmonic sum, it leads to

$$H_n = \ln n + \gamma + \frac{1}{2n} - R_n,$$

where

$$\frac{1}{12(n+1)^2} \leqslant R_n \leqslant \frac{1}{12(n-1)^2}.$$

However, we can do even better by repeating the integration by parts and using the *Bernoulli polynomials* to select successive antiderivatives. The Bernoulli polynomials are usually defined to be the polynomials $B_n(x)$ appearing in the expansion

$$\frac{te^{xt}}{e^t - 1} = \sum_{n=0}^{\infty} B_n(x) \frac{t^n}{n!},$$

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but an equivalent definition, more useful for our present purposes, is as follows. Put $B_0(x) = 1$, then

$$B_n(x) = n\int_0^x B_{n-1}(t)\,dt + B_n,$$

where the constant $B_n = B_n(0)$ is chosen to ensure that $\int_0^1 B_n(x)\,dx = 0$. The numbers B_n are called the *Bernoulli numbers*. So $B_1(x) = x - \frac{1}{2}$, the factor appearing in (5). Next, $B_2(x) = x^2 - x + B_2$, where $\frac{1}{3} - \frac{1}{2} + B_2 = 0$, hence $B_2 = \frac{1}{6}$, so that

$$B_2(x) = x^2 - x + \tfrac{1}{6}.$$

Continuing, we find by easy calculations

$$B_3(x) = x^3 - \tfrac{3}{2}x^2 + \tfrac{1}{2}x = x\left(x - \tfrac{1}{2}\right)(x - 1),$$

$$B_4(x) = x^4 - 2x^3 + x^2 - \tfrac{1}{30} = x^2(x-1)^2 - \tfrac{1}{30},$$

$$B_5(x) = x^5 - \tfrac{5}{2}x^4 + \tfrac{5}{3}x^3 - \tfrac{1}{6}x = x\left(x - \tfrac{1}{2}\right)(x-1)\left(x^2 - x - \tfrac{1}{3}\right).$$

Note that $B_4 = -\frac{1}{30}$ and $B_3 = B_5 = 0$. The stated factorisation of $B_5(x)$ is not hard, once it is recognised that it is zero at 0, $\frac{1}{2}$ and 1.

The Bernoulli numbers have many applications. The best-known ones are explicit formulae for $\sum_{r=1}^{n} r^m$ [2, p. 90] and $\zeta(2n)$ [3, p. 283]. This notation is now standard, but variations will be found in older books, for example B_n where we have $(-1)^{n-1}B_{2n}$.

For the cases just listed, it is clear that $B_n(1-x)$ equals $B_n(x)$ when n is even, and $-B_n(1-x)$ when n is odd. Another way of stating this is $B_n\left(\frac{1}{2} + y\right) = (-1)^n B_n\left(\frac{1}{2} - y\right)$: the functions are even, or odd, with respect to the point $\frac{1}{2}$. These properties actually hold for all n; they are an important characteristic of the Bernoulli polynomials. In particular, $B_n(1) = B_n$ for even n, and $B_3(1) = B_5(1) = 0$.

By the fundamental theorem of calculus, $B_n'(x) = nB_{n-1}(x)$. We integrate repeatedly by parts, using $\frac{1}{n}B_n(x)$ as the antiderivative of $B_{n-1}(x)$. We assume that $f(x)$ has enough derivatives for the formulae stated. The outcome of the first two stages is as follows:

Theorem 3:

$$T(f) - J(f) = \tfrac{1}{12}\left[f'(1) - f'(0)\right] + R_2, \tag{10}$$

where

$$R_2 = -\tfrac{1}{2}\int_0^1 B_2(x)f''(x)\,dx = \tfrac{1}{6}\int_0^1 B_3(x)f^{(3)}(x)\,dx. \tag{11}$$

Further,

$$T(f) - J(f) = \tfrac{1}{12}\left[f'(1) - f'(0)\right] - \tfrac{1}{720}\left[f^{(3)}(1) - f^{(3)}(0)\right] + R_4,$$

where

$$R_4 = -\frac{1}{4!}\int_0^1 B_4(x)f^{(4)}(x)\,dx = \frac{1}{5!}\int_0^1 B_5(x)f^{(5)}(x)\,dx. \tag{13}$$

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Proof: Integrate by parts in (5), using $\frac{1}{2}B_2(x)$ as the antiderivative of $x - \frac{1}{2}$. Since $B_2(0) = B_2(1) = \frac{1}{6}$, we obtain

$$T(f) - J(f) = \left[\tfrac{1}{2}B_2(x)f'(x)\right]_0^1 - \tfrac{1}{2}\int_0^1 B_2(x)f''(x)\,dx$$

$$= \tfrac{1}{2}\left[f'(1) - f'(0)\right] - \tfrac{1}{2}\int_0^1 B_2(x)f''(x)\,dx.$$

In the same way, since $B_3(0) = B_3(1) = 0$,

$$\int_0^1 B_2(x)f''(x) = \left[\tfrac{1}{3}B_3(x)f''(x)\right]_0^1 - \tfrac{1}{3}\int_0^1 B_3(x)f^{(3)}(x)\,dx$$

$$= -\tfrac{1}{3}\int_0^1 B_3(x)f^{(3)}(x)\,dx.$$

This establishes (10) and (11). Repeating the process, using $B_4(0) = B_4(1) = -\frac{1}{30}$, we obtain

$$\int_0^1 B_3(x)f^{(3)}(x)\,dx = \left[\tfrac{1}{4}B_4(x)f^{(3)}(x)\right]_0^1 - \tfrac{1}{4}\int_0^1 B_4(x)f^{(4)}(x)\,dx$$

$$= -\tfrac{1}{120}\left[f^{(3)}(1) - f^{(3)}(0)\right] - \tfrac{1}{4}\int_0^1 B_4(x)f^{(4)}(x)\,dx$$

and then, since $B_5(0) = B_5(1) = 0$,

$$\int_0^1 B_4(x)f^{(4)}(x)\,dx = -\tfrac{1}{5}\int_0^1 B_5(x)f^{(5)}(x)\,dx.$$

Substituted into (10) and (11), this gives (12) and (13).

This is the promised truncated version of Euler-Maclaurin summation. The full version will be described briefly below, but we do not need it for present purposes. Instead, what we now need is a further result ensuring that R_2 and R_4 are either positive or negative, thereby delivering upper and lower bounds. The underlying principle is pleasantly simple, as we now demonstrate.

Lemma: Suppose that f and g are two functions on $[0, 1]$ such that $f(x)$ is increasing and $g(1 - x) = -g(x)$ for $0 \leqslant x \leqslant 1$, and $g(x) \geqslant 0$ for $0 \leqslant x \leqslant \frac{1}{2}$. Then

$$\int_0^1 f(x)g(x)\,dx \leqslant 0.$$

If $g(x) \leqslant 0$ on $[0, \frac{1}{2}]$, then the inequality reverses.

Proof: The substitution $x = 1 - y$ gives

$$\int_{1/2}^1 f(x)g(x)\,dx = \int_0^{1/2} f(1 - y)\left[-g(y)\right]dy,$$

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hence, if $g(x) \geqslant 0$ on $[0, \frac{1}{2}]$

$$\int_0^1 f(x)\,g(x)\,dx = \int_0^{1/2} \left[f(x) - f(1-x)\right] g(x)\,dx \leqslant 0,$$

since $f(x) - f(1-x) \leqslant 0$ for $0 \leqslant x \leqslant \frac{1}{2}$.

Applied to (5), this reproduces the fact that if $f'(x)$ is increasing, then $T(f) \geqslant J(f)$, as we saw from (9).

As already mentioned, $B_n(1-x) = -B_n(x)$ for $n = 3$ and $n = 5$. Also, for $0 \leqslant x \leqslant \frac{1}{2}$, $B_3(x) \geqslant 0$, since it is a product of x and two negative factors, while $B_5 \leqslant 0$, since $x^2 - x - \frac{1}{3} < 0$. So we can use Lemma 1 to convert (10) and (12) into inequalities, as follows:

Theorem 4: If $f^{(3)}(x)$ and $f^{(5)}(x)$ are increasing, then

$$T(f) - J(f) = \frac{1}{12}\left[f'(1) - f'(0)\right] - \delta(f), \tag{14}$$

where

$$0 \leqslant \delta(f) \leqslant \tfrac{1}{720}\left[f^{(3)}(1) - f^{(3)}(0)\right]. \tag{15}$$

Proof: By the Lemma, under these assumptions, $R_2 \leqslant 0$ and $R_4 \geqslant 0$, so that

$$\tfrac{1}{12}\left[f'(1) - f'(0)\right] - \tfrac{1}{720}\left[f^{(3)}(1) - f^{(3)}(0)\right] \leqslant T(f) - J(f) \leqslant \tfrac{1}{12}\left[f'(1) - f'(0)\right], \tag{16}$$

which equates to (14) and (15).

If $f^{(3)}(x)$ and $f^{(5)}(x)$ are decreasing, then the inequalities in (16) reverse, and it is more natural to restate (14) and (15) as follows:

$$T(f) - J(f) = \tfrac{1}{12}\left[f'(1) - f'(0)\right] + \delta(f), \tag{17}$$

where

$$0 \leqslant \delta(f) \leqslant \tfrac{1}{720}\left[f^{(3)}(0) - f^{(3)}(1)\right]. \tag{18}$$

Now let us extend these results to other intervals. In Theorem 3, all we have to do is replace $B_n(x)$ by $B_n\big(x - [x]\big)$, as we did in (7). But what we really want is the extension of Theorem 4. Applying it to $f(x + r)$, with $T_r(f)$ and $J_r(f)$ defined as before, we obtain:

$$T_r(f) - J_r(f) = \tfrac{1}{12}\left[f'(r+1) - f'(r)\right] - \delta_r(f), \tag{19}$$

where

$$0 \leqslant \delta_r(f) \leqslant \tfrac{1}{720}\left[f^{(3)}(r+1) - f^{(3)}(r)\right]. \tag{20}$$

We now add these statements for $1 \leqslant r \leqslant n-1$. By cancellation, $\sum_{r=1}^{n-1}\left[f'(r+1) - f(r)\right]$ telescopes to $f'(n) - f'(1)$, so we obtain:

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Theorem 5: If $f^{(3)}(x)$ and $f^{(5)}(x)$ are increasing, then for all $n \geqslant 2$,

$$S_n^*(f) - I_n(f) = \tfrac{1}{12}\left[f'(n) - f'(1)\right] - \sum_{r=1}^{n-1} \delta_r(f), \tag{21}$$

where $\delta_r(f)$ satisfies (20). (Also, (21) holds for $n = 1$, with both sides 0.)

If $f^{(3)}(x)$ and $f^{(5)}(x)$ are decreasing, this is modified in the way seen in (17) and (18).

It is now a short step, not just to Theorem 1, but to the following more general result:

Theorem 6: Suppose that $f(x)$ and all its derivatives tend to 0 as $x \to \infty$, and that $f^{(3)}(x)$ and $f^{(5)}(x)$ are increasing. Then $S_n(f) - I_n(f)$ tends to a limit L as $n \to \infty$, and for all $n \geqslant 1$,

$$S_n(f) = I_n(f) + L + \tfrac{1}{2}f(n) + \tfrac{1}{12}f'(n) + r_n(f), \tag{22}$$

where

$$0 \leqslant r_n(f) \leqslant -\tfrac{1}{720}f^{(3)}(n). \tag{23}$$

Proof: We apply (21). Since $\sum_{r=1}^{n-1}\left[f^{(3)}(r+1) - f^{(3)}(r)\right] = f^{(3)}(n) - f^{(3)}(1)$ and $f^{(3)}(n)$ tends to zero, it follows from (20) that $\sum_{r=1}^{\infty} \delta_r(f)$ is convergent. Hence $S_n^*(f) - I_n(f) \to L^*$ as $n \to \infty$, where

$$L^* = -\tfrac{1}{12}f'(1) - \sum_{r=1}^{\infty} \delta_r(f).$$

Further, by subtraction,

$$S_n^*(f) - I_n(f) - L^* = \tfrac{1}{12}f'(n) + r_n(f),$$

where

$$r_n(f) = \sum_{r=n}^{\infty} \delta_r(f) \leqslant \tfrac{1}{720}\sum_{r=n}^{\infty}\left[f^{(3)}(r+1) - f^{(3)}(r)\right] = -\tfrac{1}{720}f^{(3)}(n),$$

also $r_n(f) \geqslant 0$. Now $S_n(f) = S_n^*(f) + \tfrac{1}{2}f(1) + \tfrac{1}{2}f(n)$, so (22) holds with $L = L^* + \tfrac{1}{2}f(1)$.

Theorem 1 is the case $f(x) = 1/x$. We just need to insert the specific values $I_n(f) = \ln n$, $f'(x) = -1/x^2$ and $f^{(3)}(x) = -6/x^4$, and note that the odd-numbered derivatives are negative, and also increasing because the even-numbered derivatives are positive.

Theorem 6 can equally be applied to $1/x^p$ for any p in (0, 1): there is an 'Euler-type' constant L_p for each p. We leave it to the reader to write out the formulae explicitly. Just taking $n = 1$, we obtain $L_p = \frac{1}{2} + \frac{p}{12} - \delta_p$, where $0 \leqslant \delta_p \leqslant \frac{1}{720}p(p+1)(p+2)$. This can be compared with the estimation of L_p (in different notation) in [4].

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Theorem 6 still applies if the derivatives are increasing only for large enough x, say for $x \geqslant 0$: then (23) holds for $n \geqslant x_0$. A case where this occurs is $f(x) = (\ln x)^k / x$ for $k \geqslant 1$; the resulting constant is called the *Stieltjes constant* γ_k. Taking $n = 10$, we find $\gamma_1 = -0.07282$ to five d.p.

More harmonic sums

We describe two further applications to sums derived from the harmonic series.

Theorem 7: Let $U_n = \sum_{r=1}^{n} \dfrac{1}{2r-1}$. Then

$$U_n = \tfrac{1}{2}\ln n + \ln 2 + \tfrac{1}{2}\gamma + \frac{1}{48n^2} + s_n,$$

where

$$-\frac{1}{240n^4} \leqslant s_n \leqslant \frac{1}{480n^4}.$$

Proof: Note that $U_n = H_{2n} - \sum_{r=1}^{n} \frac{1}{2r} = H_{2n} - \frac{1}{2}H_n$. By (1),

$$H_{2n} = \ln 2n + \gamma + \frac{1}{4n} - \frac{1}{48n^2} + r_{2n}$$

and

$$\tfrac{1}{2}H_n = \tfrac{1}{2}\ln n + \tfrac{1}{2}\gamma + \frac{1}{4n} - \frac{1}{24n^2} + \tfrac{1}{2}r_n,$$

so

$$U_n = \tfrac{1}{2}\ln n + \ln 2 + \tfrac{1}{2}\gamma + \frac{1}{48n^2} + r_{2n} - \tfrac{1}{2}r_n.$$

Since $0 \leqslant r_{2n} \leqslant \frac{1}{480n^4}$ and $0 \leqslant \frac{1}{2}r_n \leqslant \frac{1}{240n^4}$, the statement follows.

Theorem 8: Let $L_n = \sum_{r=n+1}^{2n} \frac{1}{r}$. Then

$$L_n = \ln 2 - \frac{1}{4n} + \frac{1}{16n^2} - t_n, \tag{24}$$

where

$$0 \leqslant t_n \leqslant \frac{1}{128n^4}.$$

Proof: Combining (19) for $n \leqslant r \leqslant 2n-1$, we have

$$\tfrac{1}{2}f(n) + \sum_{r=n+1}^{2n-1} f(r) + \tfrac{1}{2}f(2n) = \int_n^{2n} f(x)\,dx + \tfrac{1}{12}\left|f'(2n) - f'(n)\right| - \sum_{r=n}^{2n-1} \delta_r(f).$$

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With $f(x) = 1/x$, the left-hand side is $L_n + \frac{1}{2n} - \frac{1}{4n} = L_n + \frac{1}{4n}$. So

$$L_n + \frac{1}{4n} = \ln 2 + \frac{1}{12n^2} - \frac{1}{12(2n)^2} - \sum_{r=n}^{2n-1} \delta_r(f)$$

$$= \ln 2 + \frac{1}{16n^2} - \sum_{r=n}^{2n-1} \delta_r(f),$$

and by (20),

$$0 \leqslant \sum_{r=n}^{2n-1} \delta_r(f) \leqslant \frac{1}{120}\left(\frac{1}{n^4} - \frac{1}{(2n)^4}\right) = \frac{1}{128n^4}.$$

For example, this gives $L_{100} = H_{200} - H_{100} = 0.6906534$ to seven d.p. For this, we needed to know $\ln 2$, but not γ. Viewed the other way round, we can regard (24) as giving bounds for $\ln 2$: with n taken to be only 4, these bounds are 0.693117 and 0.693148.

Stirling's formula

A great deal has been written about Stirling's formula. Here we just mention two *Gazette* articles, [5], which contains an interesting historical survey, and [6], which addresses the enhanced version we are considering, but by a different method.

In common with most proofs of Stirling's formula, we concentrate on showing that (3) holds for *some* constant c; the evaluation of c (and C) can then be achieved using the Wallis product: see, for example, [5]. We will not repeat this part of the proof here.

The proof is exactly similar to Theorem 6, except that the odd-numbered derivatives are now decreasing.

Proof of Theorem 2: Take $f(x) = \ln x$. Then $f'(x) = 1/x$ and $f^{(3)}(x) = 2/x^3$. We apply Theorem 5, suitably modified for the case where $f^{(3)}(x)$ and $f^{(5)}(x)$ are decreasing. We obtain

$$\sum_{r=1}^{n} \ln r = S_n^*(f) + \tfrac{1}{2}\ln n$$

$$= \tfrac{1}{2}\ln n + \int_1^n \ln x\,dx + \frac{1}{12}\left(\frac{1}{n} - 1\right) + \sum_{r=1}^{n-1} \delta_r(f)$$

$$= \left(n + \tfrac{1}{2}\right)\ln n - n + 1 - \frac{1}{12} + \frac{1}{12n} + \sum_{r=1}^{n-1} \delta_r(f),$$

where

$$0 \leqslant \delta_r(f) \leqslant \frac{1}{360}\left(\frac{1}{r^3} - \frac{1}{(r+1)^3}\right).$$

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Now $\sum_{r=1}^{\infty} \delta_r(f)$ is convergent, so

$$\sum_{r=1}^{n} \ln r - \left(n + \tfrac{1}{2}\right) \ln n - \frac{1}{12n} = c - q_n,$$

where

$$c = 1 - \tfrac{1}{12} + \sum_{r=1}^{\infty} \delta_r(f)$$

and

$$q_n = \sum_{r=1}^{\infty} \delta_r(f) \leqslant \frac{1}{360n^3}.$$

There is a generalised version of Stirling's formula applying to the gamma function [7, p. 21-22]. A simple method, again using (19) and (20) for the case $1/x$, is presented in a companion note [8].

Estimating the sum of a convergent series

Suppose that $f(x)$ is positive and decreasing, and the series $\sum_{n=1}^{\infty} f(n)$ is convergent, with sum $S(f)$. Let $S_n(f) = \sum_{r=1}^{n} f(r)$. How close is $S_n(f)$ to $S(f)$? The difference is $\sum_{r=n+1}^{\infty} f(r)$. In some sense, this is approximated by $\int_n^{\infty} f(x)\,dx$. We can turn this into an accurate statement using Theorem 5; this is actually rather simpler than Theorem 6, because there is no step corresponding to the introduction of the constant L.

Theorem 9: Suppose that $f(x) \geqslant 0$ on $[1, \infty)$ and that $\sum_{n=1}^{\infty} f(n)$ is convergent, with sum $S(f)$. Suppose also that $f^{(n)}(x) \to 0$ as $x \to \infty$ for all n, and that the even-numbered derivatives are positive. Then, for each $n \geqslant 1$,

$$S(f) = S_{n-1}(f) + \tfrac{1}{2} f(n) + \int_n^{\infty} f(x)\,dx - \tfrac{1}{12} f'(n) - r_n(f),$$

where

$$0 \leqslant r_n(f) \leqslant -\tfrac{1}{720} f^{(3)}(n).$$

Proof: Continue to write $T_r(f) = \frac{1}{2} f(r) + \frac{1}{2} f(r+1)$. Then

$$\sum_{r=n}^{\infty} T_r(f) = \tfrac{1}{2} f(n) + \sum_{r=n+1}^{\infty} f(r).$$

The odd-numbered derivatives are increasing. Adding together (19) for all $r \geqslant n$, we obtain

$$\sum_{r=n}^{\infty} T_r(f) = \int_n^{\infty} f(x)\,dx - \frac{1}{12} f'(n) - r_n(f),$$

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where

$$r_n(f) = \sum_{r=n}^{\infty} \delta_r(f),$$

so that by (20)

$$0 \leqslant r_n(f) \leqslant \tfrac{1}{720} \sum_{r=n}^{\infty} \left[f^{(3)}(r+1) - f^{(3)}(r)\right] = -\tfrac{1}{720} f^{(3)}(n).$$

To obtain $S(f)$, we now add $S_{n-1}(f) + \frac{1}{2}f(n)$.

We record the particular case given by $f(x) = 1/x^2$. Of course, it is well known that $\sum_{n=1}^{\infty} 1/n^2 = \pi^2/6$. However, our present concern is simply to give bounds for the whole sum having added n terms. Now $\int_n^{\infty} f(x) = \frac{1}{n}$, while $f'(x) = -2/x^3$ and $f^{(3)}(x) = -24/x^5$, so Theorem 8 gives:

Corollary: Let $S = \sum_{n=1}^{\infty} \frac{1}{n^2}$. Then

$$S = \sum_{r=1}^{n-1} \frac{1}{r^2} + \frac{1}{n} + \frac{1}{2n^2} + \frac{1}{6n^3} - r_n,$$

where

$$0 \leqslant r_n \leqslant \frac{1}{30x^5}.$$

Taking $n = 5$ (that is, only adding 5 terms), this gives bounds 1.6449337 and 1.6449444 to seven d.p.; compare the actual value 1.6449341.

We again leave it to the reader to write out the statement for $\sum_{n=1}^{\infty} 1/n^p$.

Alternative proofs by power series

For Theorem 1, we used (19) and (20) for the specific case $f(x) = 1/x$. Explicitly, this says

$$\frac{1}{2r} + \frac{1}{2(r+1)} = \ln(r+1) - \ln r + \frac{1}{12}\left(\frac{1}{r^2} - \frac{1}{(r+1)^2}\right) - \delta_r, \qquad (25)$$

where $0 \leqslant \delta_r \leqslant \frac{1}{120}\left(\frac{1}{r^4} - \frac{1}{(r+1)^4}\right)$. We indicate briefly a direct proof of (25) based on power series; the method can be traced at least to [7, p. 21]. We have $\ln(r+1) - \ln r = \ln\left(1 + 1/r\right)$ and $1 + 1/r = (1+x)/(1-x)$, where $x = 1/(2r+1)$. Also,

$$\frac{1}{2r} = \frac{x}{1-x}, \qquad \frac{1}{2(r+1)} = \frac{x}{1+x}.$$

Using these identities, we express $\ln\left(1 + 1/r\right)$ and $r^{-k} - (r+1)^{-k}$ (for $k = 1, 2, 4$) as power series in x. After some manipulation, term-by-term comparison establishes (25). Similar methods can be used to prove (19) and

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(20) for the cases $f(x) = \ln x$ and $f(x) = 1/x^2$, which we used in Theorems 2 and 9, but of course each case has to be proved separately.

Further steps: the full version of Euler-Maclaurin summation

Of course, the process in Theorem 3 can be continued. We describe the outcome briefly for any readers who are interested. One needs to know the following facts about the Bernoulli numbers and polynomials, which we could simply spot in the first few cases, but now need to be proved: this is mostly straightforward by induction (e.g. [3, chapter 8]).

$B_{2k}(1 - x) = B_{2k}(x)$ and $B_{2k+1}(1 - x) = -B_{2k+1}(x)$;

$B_{2k} < 0$ for k even and $B_{2k} > 0$ for k odd;

$B_{2k+1} = 0$;

$B_{2k+1}(x)$ is negative on $\left[0, \frac{1}{2}\right]$ for k even, positive for k odd.

After k iterations, the statement is

$$T(f) - J(f) = \sum_{j=1}^{k} \frac{B_{2j}}{(2j)!}\left[f^{(2j-1)}(1) - f^{(2j-1)}(0)\right] + R_{2k},$$

where

$$R_{2k} = -\frac{1}{(2k)!}\int_0^1 B_{2k}(x) f^{(2k)}(x)\,dx = \frac{1}{(2k+1)!}\int_0^1 B_{2k+1}(x) f^{(2k+1)}(x)\,dx.$$

Further, if the odd-numbered derivatives are increasing, then $R_{2k} \geqslant 0$ if k is even, and $R_{2k} \leqslant 0$ if k is odd. The statements can then be combined over successive intervals $[r, r + 1]$ as before.

The Bernoulli numbers satisfy $\sum_{r=0}^{n-1} \binom{n}{r} B_r = 0$, from which one can calculate them successively. In particular, we find $B_6 = \frac{1}{42}$, $B_8 = -\frac{1}{30}$, $B_{10} = \frac{5}{66}$. The case $k = 3$ gives the next stage beyond Theorem 4: if the odd-numbered derivatives are increasing, then

$$T(f) - J(f) \leqslant \tfrac{1}{12}\left[f'(1) - f'(0)\right] - \tfrac{1}{720}\left[f^{(3)}(1) - f^{(3)}(0)\right] + \tfrac{1}{6!42}\left[f^{(5)}(1) - f^{(5)}(0)\right].$$

For the harmonic sum, this gives

$$H_n = \ln n + \gamma + \frac{1}{2n} - \frac{1}{12n^2} + \frac{1}{120n^4} - t_n,$$

where

$$0 \leqslant t_n \leqslant \frac{1}{252n^6},$$

and for Stirling's formula it gives

$$\ln n! = \left(n + \tfrac{1}{2}\right)\ln n - n + c + \frac{1}{12n} - \frac{1}{360n^3} + u_n,$$

where

$$0 \leqslant u_n \leqslant \frac{1}{1260n^5}.$$

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This, and even a further term, is given in [6]. The method uses power series and some fairly heavy algebra, and readers may care to compare it with the method described here.

Given the values of the Bernoulli numbers, it is easy to write down further terms in the Euler-Maclaurin formula. One might suppose that the process generates ever closer approximations, and hence a convergent series, but in fact this is deceptive, because the Bernoulli numbers eventually grow large. In fact, it follows from the identity relating B_{2j} with $\zeta(2j)$ that

$$\frac{|B_{2j}|}{(2j)!} \sim \frac{2}{(2\pi)^{2j}}.$$

With $f(x) = 1/x$, we have $f^{(2j-1)}(n) = -(2j-1)!/n^{2j}$, so the magnitude of the error term in the expression for H_n is

$$\frac{|B_{2j}|}{(2j)!}\left|f^{(2j-1)}(n)\right| \sim \frac{2(2j-1)!}{(2\pi n)^{2j}},$$

which tends to infinity as $j \to \infty$, because factorials prevail over powers. Roughly speaking, the approximation is best when j is about πn, after which the error term starts growing larger again.

The Euler-Maclaurin method was used by Euler himself to calculate the first 15 digits of γ. In 1962, Knuth used it to compute 1271 digits. Since then, more sophisticated methods have been devised for the computation of γ. For a good survey, see [9].

A variant based on midpoints

Since $\ln\left(n+\frac{1}{2}\right) = \ln n + \frac{1}{2n} + O\left(\frac{1}{n^2}\right)$, it is natural, in the light of (1), to compare $H_n - \gamma$ with $\ln\left(n+\frac{1}{2}\right)$ instead of $\ln n$. De Temple and Wang [10] showed how to do this by a neat variant of Euler-Maclaurin summation. Write $K(f) = \int_{-1/2}^{1/2} f(x)\,dx$. The starting point is the following analogue of (5), in which $K(f)$ is compared with the midpoint approximation $f(0)$ instead of the trapezium expression:

$$f(0) - K(f) = \int_0^{1/2}\left(x-\tfrac{1}{2}\right)\left(f'(x) - f'(-x)\right)dx.$$

By exactly the same steps as before (some readers may care to work through the details for themselves), we arrive at the following analogue of (14):

$$f(0) - K(f) = \tfrac{1}{2}B_2\left(\tfrac{1}{2}\right)\left(f'\left(\tfrac{1}{2}\right) - f'\left(-\tfrac{1}{2}\right)\right) + \eta(f),$$

where

$$0 \leqslant \eta(f) \leqslant \frac{1}{4!}B_4\left(\tfrac{1}{2}\right)\left(f^{(3)}\left(\tfrac{1}{2}\right) - f^{(3)}\left(-\tfrac{1}{2}\right)\right),$$

in which we can insert the values $B_2\left(\frac{1}{2}\right) = -\frac{1}{12}$ and $B_4\left(\frac{1}{2}\right) = \frac{7}{240}$. For the harmonic series, the conclusion is

$$H_n = \ln\left(n+\tfrac{1}{2}\right) + \gamma + \frac{1}{24\left(n+\frac{1}{2}\right)^2} - s_n,$$

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where

$$0 \leqslant s_n \leqslant \frac{7}{960\,(n + \frac{1}{2})^4}.$$

Of course, the process can be continued: further terms are given in [10]. The numbers $B_n\left(\frac{1}{2}\right)$ do not need a new calculation: they are given by $B_n\left(\frac{1}{2}\right) = -\left(1 - \frac{1}{2^{n-1}}\right)B_n$.

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