Euler-Maclaurin summation

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Estimating sums by integrals

Consider a discrete sum of the form

$$S_{m,n}(f) = \sum_{r=m}^{n} f(r),$$

where f is a continuous function. Often there is no simple expression for $S_{m,n}(f)$, but an approximation is given by the corresponding integral

$$I_{m,n}(f) = \int_m^n f(x)\,dx,$$

which can be evaluated explicitly. The most elementary version of this procedure is as follows. Write $J_r(f) = \int_r^{r+1} f(x)\,dx$, so that $I_{m,n}(f) = \sum_{r=m}^{n-1} J_r(f)$. If $f(x)$ is non-negative and decreasing, then $f(r+1) \le f(x) \le f(r)$ for $r \le x \le r+1$, so

$$f(r+1) \le J_r(f) \le f(r). \tag{1}$$

Combining these inequalities for $m \le r \le n-1$, we obtain $S_{m+1,n}(f) \le I_{m,n}(f) \le S_{m,n-1}(f)$, hence

$$I_{m,n}(f) + f(n) \le S_{m,n}(f) \le I_{m,n}(f) + f(m). \tag{2}$$

Rewriting (1) as $J_r(f) \le f(r) \le J_{r-1}(f)$, we can deduce the following variant:

$$I_{m,n+1}(f) \le S_{m,n}(f) \le I_{m-1,n}(f). \tag{3}$$

Of course, opposite inequalities apply for an increasing function.

We write just $S_n(f)$ for $S_{1,n}(f)$ and $I_n(f)$ for $I_{1,n}(f)$.

These inequalities extend in two ways to the infinite case. First, suppose that $f(x)$ is positive, decreasing and tends to 0 as $x \to \infty$. It follows from (2) that convergence of the series $\sum_{n=1}^{\infty} f(n)$ is equivalent to convergence of the integral $\int_1^{\infty} f(x)\,dx$: denote these by $S(f)$ and $I(f)$ respectively. Also, write $S_{m,\infty}(f)$ for $\sum_{r=m}^{\infty} f(r)$ and $I_{m,\infty}(f)$ for $\int_m^{\infty} f(x)\,dx$. Taking the limit as $n \to \infty$ in (2), we see that

$$I_{m,\infty}(f) \le S_{m,\infty}(f) \le I_{m,\infty}(f) + f(m). \tag{4}$$

while (3) gives the alternative upper bound $I_{m-1,\infty}(f)$.

The most basic application is to the series $\sum_{n=1}^{\infty} 1/n^p$, where $p > 1$: its sum defines the *Riemann zeta function* $\zeta(p)$. With $f(x) = 1/x^p$, we have $I(f) = 1/(p-1)$, hence by (4),

$$\frac{1}{p-1} \leq \zeta(p) \leq \frac{1}{p-1} + 1. \tag{5}$$

To obtain a more accurate estimation for a particular p, we first add a chosen number of terms and then use (4) to estimate the tail of the series. For example, for the case $p = 2$, (4) gives

$$\frac{1}{m} \leq \sum_{r=m}^{\infty} \frac{1}{r^2} \leq \frac{1}{m} + \frac{1}{m^2}. \tag{6}$$

In the case where the series and integral are both divergent (still with $f(x)$ decreasing and tending to 0), it follows from (1) that $S_n(f) - I_n(f)$ is decreasing, while $S_{n-1}(f) - I_n(f)$ is increasing, so both converge to a limit L as $n \to \infty$, and further $S_{n-1}(f) - I_n(f) \leq L \leq S_n(f) - I_n(f)$, equivalently

$$I_n(f) + L \leq S_n(f) \leq I_n(f) + L + f(n). \tag{7}$$

In the case $f(x) = 1/x$, L is Euler's constant γ. With the harmonic sum $\sum_{r=1}^{n} \frac{1}{n}$ denoted by H_n, (7) says

$$\log n + \gamma \leq H_n \leq \log n + \gamma + \frac{1}{n}. \tag{8}$$

In (1), J_r was estimated by constant upper and lower bounds on the interval. A closer approximation will usually be given by the trapezium rule. For this purpose, write

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

and

$$S^*_{m,n}(f) = \sum_{r=m}^{n-1} T_r(f) = \tfrac{1}{2} f(m) + \sum_{r=m+1}^{n-1} f(r) + \tfrac{1}{2} f(n), \tag{9}$$

so that

$$S_{m,n}(f) = S^*_{m,n}(f) + \tfrac{1}{2} f(n) + \tfrac{1}{2} f(m).$$

We write $S^*_n(f)$ for $S^*_{1,n}(f)$ and $S^*_{m,\infty}(f)$ for $\frac{1}{2} f(m) + \sum_{r=m+1}^{\infty} f(r)$ when the series converges.

It is geometrically compelling, and easily proved, that if f is *convex*, then $T_r(f) \geq J_r(f)$, hence $S^*_{m,n}(f) \geq I_{m,n}(f)$ (this will also follow from Proposition 3 below). This improves the lower bound in (4) to $I_{m,\infty}(f) + \frac{1}{2} f(m)$. So, for example, $\zeta(p) \geq \frac{1}{p-1} + \frac{1}{2}$.

The objective of Euler-Maclaurin summation is to give an accurate estimation of the difference $S^*_{m,n}(f) - I_{m,n}(f)$. We shall see that it is highly effective.

Euler-Maclaurin: step 1

We start with the interval $[0,1]$. Write just $T(f)$ and $J(f)$ for $T_1(f)$ and $J_1(f)$. There is a simple integral expression for $T(f) - J(f)$:.

PROPOSITION 1. *For differentiable f (with real or complex values), we have*

$$T(f) - J(f) = \int_0^1 (x - \tfrac{1}{2}) f'(x)\, dx. \tag{10}$$

Proof. Integrating by parts, we obtain

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

To translate this to the interval $[r, r+1]$, we just apply it to $f(x+r)$. To express the result, we introduce some notation which might seem unnecessary, but it is the precursor of what is to come. Write $B_1(x) = x - \frac{1}{2}$, and $\tilde{B}_1(x)$ for the 1-periodic extension of its values on $[0,1]$, so that $\tilde{B}_1(x) = B_1(x-r)$ on $[r, r+1)$. Another way to state this is: $\tilde{B}_1(x) = B_1(x - [x])$, where $[x]$ is the integer part of x.

Applying (10) to $f(x+r)$ (or just as easily, by direct integration), we obtain:

$$T_r(f) - J_r(f) = \int_r^{r+1} \tilde{B}_1(x) f'(x)\, dx.$$

Combining over successive intervals, we obtain:

THEOREM 2. *For differentiable f,*

$$S^*_{m,n}(f) - I_{m,n}(f) = \int_m^n \tilde{B}_1(x) f'(x)\, dx. \qquad \square \tag{11}$$

This is the first step of Euler-Maclaurin summation. Of course, for $S_{m,n}(f)$, we simply add $\frac{1}{2} f(m) + \frac{1}{2} f(n)$.

Note that $|\tilde{B}_1(x)| \le \frac{1}{2}$ for all x, so the right-hand side of (11) is bounded by $\frac{1}{2} \int_m^n |f'(x)| dx$.

Let us revisit (4) and (7) in the light of (11). Clearly, if $\int_1^\infty \tilde{B}_1(x) f'(x)\, dx$ is convergent, then (11) gives

$$\lim_{n\to\infty} \Big(S^*_{m,n}(f) - I_{m,n}(f) \Big) = \int_m^\infty \tilde{B}_1(x) f'(x)\, dx. \tag{12}$$

Convergence of $S(f)$ is then equivalent to convergence of $I(f)$, and when this occurs, the left-hand side of (12) becomes simply $S^*_{m,\infty}(f) - I_{m,\infty}(f)$. For $m = 1$, with $\frac{1}{2} f(1)$ added, this says:

$$S(f) = I(f) + \tfrac{1}{2} f(1) + \int_1^\infty \tilde{B}_1(x) f'(x)\, dx. \tag{13}$$

In the case when $S(f)$ and $I(f)$ diverge, (12) asserts the existence of an Euler-type constant: $S_n^*(f) - I_n(f) \to L^*$ as $n \to \infty$, where

$$L^* = \int_1^\infty \tilde{B}_1(x) f'(x)\, dx. \tag{14}$$

Now subtracting (14) from (11) (with $m = 1$), we obtain

$$S_n^*(f) = I_n(f) + L^* - \int_n^\infty \tilde{B}_1(x) f'(x)\, dx, \tag{15}$$

or equivalently, adjusted to $S_n(f)$,

$$S_n(f) = I_n(f) + L + \tfrac{1}{2} f(n) - \int_n^\infty \tilde{B}_1(x) f'(x)\, dx, \tag{16}$$

where $L = L^* + \frac{1}{2} f(1)$. The further condition $\lim_{x\to\infty} f(x) = 0$ is needed to infer $S_n(f) - I_n(f) \to L$ as $n \to \infty$,

In particular, we have the following expression for Euler's constant:

$$\gamma = \tfrac{1}{2} - \int_1^\infty \frac{\tilde{B}_1(x)}{x^2}\, dx. \tag{17}$$

All this was subject to the condition that $\int_1^\infty \tilde{B}_1(x) f'(x)\, dx$ converges. This certainly occurs if $\int_1^\infty |f'(x)|\, dx$ is convergent. In turn, a sufficient condition for this is that $f'(x)$ is of one sign for large enough x and $\lim_{x\to\infty} f(x) = 0$. However, we shall see that there are cases where $\int_1^\infty \tilde{B}_1(x) f'(x)\, dx$ converges without any of these conditions being satisfied.

Extension of the Riemann zeta function

This section is not essential: it could be omitted or deferred. It describes a well-known application of (11) to complex-valued functions (though the reader is at liberty to restrict to the real case). Following the traditional notation in this subject area, we write the complex number s as $\sigma + it$. The series $\sum_{n=1}^\infty 1/n^s$ converges, so can be taken as the definition of $\zeta(s)$, for all complex s with $\sigma > 1$, but it diverges for other s. We show how (13) can be used to extend the definition to the region $\sigma > 0$. Further extension is posssible (we return to this later), but for some purposes, including the proof of the prime number theorem, the extension to $\sigma > 0$ is quite sufficient.

Let $f(x) = 1/x^s$. For $\sigma > 1$, we have $I(f) = 1/(s-1)$. By (13),

$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} + \rho_1(s), \tag{18}$$

where

$$\rho_1(s) = -s \int_1^\infty \frac{\tilde{B}_1(x)}{x^{s+1}}\, dx. \tag{19}$$

Now $|\tilde{B}_1(x)| \le \frac{1}{2}$ for all x. Also, $|x^{s+1}| = x^{\sigma+1}$, and for $\sigma > 0$, $\int_1^\infty 1/x^{\sigma+1}\, dx$ converges, with value $1/\sigma$. So for all s with $\sigma > 0$ except $s = 1$, the integral defining $\rho_1(s)$ is convergent, and we can take (18) and (19) as the *definition* of $\zeta(s)$.

Furthermore, we have shown that $|\rho_1(s)| \le |s|/2\sigma$. When s is real, say $s = p \in (0, 1)$, this just says $|\rho_1(p)| \le \frac{1}{2}$, so the inequalities in (5) still apply (note that consequently $\zeta(p) < 0$). By convexity of $1/x^p$, we actually have $\rho_1(p) \ge 0$.

As (14) shows, $\zeta(s) - 1/(s-1)$ is actually the Euler-type constant L for $1/x^s$.

This extension would not be much use if the extended function did not have nice properties. By standard results on uniform convergence and differentiation under the integral sign, one can show that the function $\rho_1(s)$ is holomorphic (so certainly continuous) for $\sigma > 0$, hence the extended $\zeta(s)$ is holomorphic except at the point 1. A pleasant consequence of this fact, together with (16), is the following limit:

$$\lim_{s\to 1}\left(\zeta(s) - \frac{1}{s-1}\right) = \tfrac{1}{2} + \rho_1(1) = \tfrac{1}{2} - \int_1^\infty \frac{\tilde{B}_1(x)}{x^2}\, dx = \gamma.$$

For further properties of the extended function, and for computing its value, a more useful expression is found by combining with (11). It relates $\zeta(s)$ to the partial sums of the original series. Duly allowing for the half values at 1 and n, (11) gives

$$\sum_{r=1}^n \frac{1}{r^s} = \frac{1}{2} + \frac{1}{2n^s} + \frac{1}{s-1}(1 - n^{1-s}) - s\int_1^n \frac{\tilde{B}_1(x)}{x^{s+1}}\, dx.$$

Subtracting this from (18), we obtain:

$$\zeta(s) = \sum_{r=1}^{n-1} \frac{1}{r^s} + \frac{1}{2n^s} + \frac{n^{1-s}}{s-1} + \rho_n(s), \tag{20}$$

$$\rho_n(s) = -s\int_n^\infty \frac{\tilde{B}_1(x)}{x^{s+1}}\, dx.$$

This is, in fact, just a restatement of (16) for $f(x) = 1/x^s$. Further, $|\rho_n(s)| \le |s|/(2\sigma n^\sigma)$, so tends to 0 as $n \to \infty$.

A typical application is the inequality $|\zeta(1+it)| \le \log t + 2\frac{1}{2}$ for $t \ge 2$, proved as follows. Take $n = [t]$ in (20). Then $|n^{1-s}| = |n^{it}| = 1$ and $|1 + it| \le 2n$, so

$$|\zeta(1+it)| \le \sum_{r=1}^n \frac{1}{r} + \frac{1}{t} + 1 < (\log n + 1) + \tfrac{1}{2} + 1.$$

Step 2: preliminary version

Recall from (10) that $T(f)-J(f) = \int_0^1 (x-\frac{1}{2})f'(x)\,dx$. As we have seen, this expression has its uses, but when applied together with $|x-\frac{1}{2}| \le \frac{1}{2}$, it is not productive in terms of inequalities. Indeed, for a decreasing function $f(x)$, it gives

$$|T(f)-J(f)| \le \tfrac{1}{2}\int_0^1 (-f'(x))\,dx = \tfrac{1}{2}[f(0)-f(1)].$$

This is equivalent to $f(1) \le J(f) \le f(0)$, which simply reproduces (1).

Since $\int_0^1 (x-\frac{1}{2})\,dx = 0$, one senses that there must really be a good deal of cancellation in the right-hand side. An estimate capturing this cancellation is found by integrating by parts the other way round, as follows:

PROPOSITION 3. *Let f be twice differentiable. Write $A_2(x) = x - x^2$ and $\tilde{A}_2(x) = A_2(x-[x])$. Then*

$$T_r(f) - J_r(f) = \tfrac{1}{2}\int_r^{r+1} \tilde{A}_2(x)f''(x)\,dx, \tag{21}$$

$$S^*_{m,n}(f) - I_{m,n}(f) = \tfrac{1}{2}\int_m^n \tilde{A}_2(x)f''(x)\,dx. \tag{22}$$

Hence if $m_r \le f''(x) \le M_r$ on $[r,r+1]$, then

$$\tfrac{1}{12}m_r \le T_r(f) - J_r(f) \le \tfrac{1}{12}M_r. \tag{23}$$

Proof. It is enough to prove (21) for the interval $[0,1]$; as before, we then translate to $[r,r+1]$ by considering $f(x+r)$, and combine intervals to obtain (22). Integrating by parts in (10), we have

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

The inequalities (23) follow from (21), because $x-x^2 \ge 0$ on $[0,1]$ and $\int_0^1 (x-x^2)\,dx = \frac{1}{6}$. □

In particular, if $f''(x) \ge 0$ on $[r,r+1]$ (so f is convex), then $T_r(f) \ge J_r(f)$, as mentioned earlier. Also, a sufficient condition for $\lim_{n\to\infty}[S^*_n(f) - I_n(f)]$ to exist (as in (12)) is convergence of $\int_1^\infty |f''(x)|\,dx$. This is satisfied, for example, by $\log x$ (compare the conditions discussed in relation to (12)).

We spell out a typical application of Proposition 3.

COROLLARY 3.1. *Suppose that* $f'(x) \le 0$, $f''(x) \ge 0$ *and* $f^{(3)}(x) \le 0$ *for all* $x \ge 1$, *and* $\lim_{x\to\infty} f'(x) = 0$. *Then*

$$-\tfrac{1}{12}f'(m+1) \le \lim_{n\to\infty}\left(S^*_{m,n}(f) - I_{m,n}(f)\right) \le -\tfrac{1}{12}f'(m-1). \tag{24}$$

Proof. Under these conditions, the stated limit exists, and equates to $\sum_{r=m}^{\infty}[T_r(f) - J_r(f)]$. Denote it by $R_m(f)$. In the notation of Proposition 3, we have $m_r = f''(r+1)$ and $M_r = f''(r)$, so $\frac{1}{12}\sum_{r=m+1}^{\infty} f''(r) \le R_m(f) \le \frac{1}{12}\sum_{r=m}^{\infty} f''(r)$. Now by (4), $\sum_{r=m}^{\infty} f''(r) \le I_{m-1,\infty}(f'') = -f'(m-1)$ and similarly $\sum_{r=m+1}^{\infty} f''(r) \ge -f'(m+1)$. This proves (24). □

For the tail of the series $\sum_{n=1}^{\infty} 1/n^2$, with $f(x) = 1/x^2$, this gives

$$\frac{1}{m} + \frac{1}{6(m+1)^3} \le S^*_{m,\infty}(f) \le \frac{1}{m} + \frac{1}{6(m-1)^3}. \tag{25}$$

Compare this with (6): the difference between the bounds is asymptotically $\frac{1}{m^4}$. However, we can do even better by repeating the integration by parts using the *Bernoulli polynomials* to select successive antiderivatives. This is the basic principle of Euler-Maclaurin summation. In particular, $A_2(x)$ will be replaced by another antiderivative of $x - \frac{1}{2}$, to be denoted by $B_2(x)$.

The Bernoulli polynomials and numbers

The Bernoulli polynomials are usually defined to be the polynomials $B_n(x)$ appearing in the expansion

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

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 $B_1(x) = x + B_1$, where $\frac{1}{2} + B_1 = 0$, hence $B_1 = -\frac{1}{2}$ and $B_1(x) = x - \frac{1}{2}$ (agreeing with the notation adopted earlier). 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

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

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

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

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.

This notation is now standard, but variations will be found in older books, for example B_n where we have $(-1)^{n-1}B_{2n}$.

Note that by the fundamental theorem of calculus, $B_n'(x) = nB_{n-1}(x)$.

There are numerous identites relating to the Bernoulli polynomials, but here we will strictly limit our account to the properties needed for Euler-Maclaurin summation. The reader is at liberty to defer the proofs to another day. For many applications, these properties are only needed for the first few cases (say as far as $B_5(x)$), and they can be simply spotted from the explicit formulae given above.

LEMMA 1. *Suppose that $\int_0^1 f(x)\,dx = 0$ and $f(1-x) = \varepsilon f(x)$, where ε is 1 or -1. Let $F(x) = \int_0^x f(t)\,dt$. Then*

$$F(1-x) = -\varepsilon F(x).$$

Proof. Since $\int_0^1 f(x)\,dx = 0$, we have

$$F(1-x) = \int_0^{1-x} f(t)\,dt = -\int_{1-x}^1 f(t)\,dt.$$

Now substituting $t = 1-u$, we have

$$F(1-x) = -\int_0^x f(1-u)\,du = -\varepsilon \int_0^x f(u)\,du = -\varepsilon F(x). \qquad \square$$

PROPOSITION 4. *For all $n \geq 1$, we have $B_{2n}(1-x) = B_{2n}(x)$ and $B_{2n+1}(1-x) = -B_{2n+1}(x)$. In particular, $B_{2n}(1) = B_{2n}(0) = B_{2n}$. Also, $B_{2n+1}(x)$ is zero at 0, $\frac{1}{2}$ and 1.*

Proof. We prove the first statement by induction and show that the second one follows. Clearly, $B_2(1-x) = B_2(x)$. Assume, for some $n \geq 1$, that $B_{2n}(1-x) = B_{2n}(x)$. Let $F(x) = \int_0^x B_{2n}(t)\,dt$. By Lemma 1, $F(1-x) = -F(x)$. This implies that $\int_0^1 F(x)\,dx = 0$ (substitute $x = 1-y$ again). By the way $B_{2n+1}(x)$ was defined, it now follows that $B_{2n+1} = 0$ and $B_{2n+1}(x) = (2n+1)F(x)$. Hence $B_{2n+1}(1-x) = -B_{2n+1}(x)$. This implies that $B_{2n+1}(1)$ and $B_{2n+1}(\frac{1}{2})$ are both 0. By Lemma 1 again, we now have

$$\int_0^{1-x} B_{2n+1}(t)\,dt = \int_0^x B_{2n+1}(t)\,dt,$$

and hence $B_{2n+2}(1-x) = B_{2n+2}(x)$. $\square$

PROPOSITION 5. *If n is even, then:*

(i) $B_{2n-1}(x) > 0$ *on* $(0, \frac{1}{2})$,

(ii) $B_{2n} < 0$ *and* $B_{2n} < B_{2n}(x) \leq B_{2n}(\frac{1}{2})$ *on* $(0, 1)$.

The opposite inequalities hold if n is odd.

Proof. From the expressions above, it is clear that $B_1(x) < 0$ and $B_3(x) > 0$ on $(0, \frac{1}{2})$. For induction, assume (i) for a certain even n. We show that (ii) follows. By (i), $B'_{2n}(x) = 2nB_{2n-1}(x) > 0$ on $(0, \frac{1}{2})$, so $B_{2n}(x)$ is strictly increasing on $[0, \frac{1}{2}]$, hence $B_{2n} = B_{2n}(0) < B_{2n}(x) \leq B_{2n}(\frac{1}{2})$ on $(0, \frac{1}{2}]$. Since $B_{2n}(1-x) = B_{2n}(x)$, these inequalities actually apply on $(0, 1)$. Hence also $B_{2n} < \int_0^1 B_{2n}(x)\, dx = 0$, and similarly $B_{2n}(\frac{1}{2}) > 0$.

So for a certain x_0 in $(0, \frac{1}{2})$, $B_{2n}(x_0) = 0$, also $B_{2n}(x) < 0$ on $(0, x_0)$ and $B_{2n}(x) > 0$ on $(x_0, \frac{1}{2})$. Hence $B_{2n+1}(x)$ is strictly decreasing on $(0, x_0)$ and strictly increasing on $(x_0, \frac{1}{2})$. Since $B_{2n+1}(\frac{1}{2}) = 0$, we have $B_{2n+1}(x) < 0$ on $(0, \frac{1}{2})$. Repetition of the reasoning shows that $B_{2n+3}(x) > 0$ on $(0, \frac{1}{2})$. $\square$

The even and odd cases can be combined by stating, for example, $(-1)^{n-1}B_{2n} > 0$.

PROPOSITION 6. *For all x,*

$$B_n(x) = \sum_{r=0}^{n} \binom{n}{r} B_r x^{n-r}. \tag{26}$$

In particular,

$$\sum_{r=0}^{n-1} \binom{n}{r} B_r = 0. \tag{27}$$

Proof. Identity (26) holds for $n = 1$, since $B_1(x) = x - \frac{1}{2} = B_0 x + B_1$. Assume (26) for n. From the defining formula, we see that the coefficient of x^{n-r+1} in $B_{n+1}(x)$ is

$$(n+1)\binom{n}{r}\frac{B_r}{n-r+1} = B_r\binom{n+1}{r}.$$

Also, the constant term is B_{n+1}. So (26) holds for $n+1$. Identity (27) follows by taking $x = 1$ and cancelling the term B_n, since $B_n(1) = B_n$. $\square$

Formula (27) enables us to calculate B_n successively. The next few are $B_6 = \frac{1}{42}$, $B_8 = -\frac{1}{30}$, $B_{10} = \frac{5}{66}$, $B_{12} = -\frac{691}{2730}$, $B_{14} = \frac{7}{6}$.

The next result will not be needed until our final section.

PROPOSITION 7. *For all x,*

$$B_n(2x) = 2^{n-1}\Big(B_n(x) + B_n(x+\tfrac{1}{2})\Big). \tag{28}$$

In particular,

$$B_n(\tfrac{1}{2}) = -\Big(1 - \frac{1}{2^{n-1}}\Big)B_n. \tag{29}$$

Proof. It is easily checked that (28) holds for $n = 1$ Assume it for $n-1$. Let

$$F_n(x) = B_n(2x) - 2^{n-1}\Big(B_n(x) + B_n(x+\tfrac{1}{2}\Big).$$

Since $B_n'(x) = nB_{n-1}(x)$, we have $F_n'(x) = 2nF_{n-1}(x) = 0$, so $F_n(x)$ is constant, say c_n. Now

$$\int_0^{1/2} F_n(x)\,dx = \tfrac{1}{2}\int_0^1 B_n(y)\,dy - 2^{n-1}\int_0^1 B_n(x)\,dx = 0.$$

Hence $c_n = 0$. The case $x = 0$ gives (29). □

With Proposition 5(ii), this gives at once:

COROLLARY 7.1. *We have $|B_{2n}(x)| \le |B_{2n}|$ for $0 \le x \le 1$.* □

The Bernoulli numbers appear in the explicit formula for $\sum_{r=1}^n r^p$: later we will show how this can be derived from Euler-Maclaurin summation. They also appear in the following expression for $\zeta(2n)$:

$$\zeta(2n) = (-1)^{n-1}\frac{B_{2n}}{2(2n)!}(2\pi)^{2n}.$$

We will not prove this identity here (see, for example, [AAR, p. 12]), but we note that since $\zeta(2n) \to 1$ as $n \to \infty$, it implies that

$$|B_{2n}| \sim \frac{2(2n)!}{(2\pi)^{2n}} \quad \text{as } n \to \infty,$$

so that after a few small values, $|B_{2n}|$ tends rapidly to infinity. (For example, we find that already $B_{30} > 6 \times 10^8$.)

The general Euler-Maclaurin formula

We are now, at last, ready to present the full version of Euler-Maclaurin summation. Starting with (10), we will integrate repeatedly by parts, using $\frac{1}{n}B_n(x)$ as the antiderivative of $B_{n-1}(x)$, assuming that $f(x)$ has enough derivatives for the formulae stated. Before proceeding to the general formula, we describe the first two steps.

Integrate by parts in (10), using $\frac{1}{2}B_2(x)$ as the antiderivative of $x - \frac{1}{2}$. Since $B_2(0) = B_2(1) = B_2$, we obtain

$$\begin{aligned} T(f) - J(f) &= \left[\tfrac{1}{2}B_2(x)f'(x)\right]_0^1 - \tfrac{1}{2}\int_0^1 B_2(x)f''(x)\,dx \\ &= \tfrac{1}{2}B_2\Big(f'(1) - f'(0)\Big) + R_2, \end{aligned}$$

where $R_2 = -\frac{1}{2}\int_0^1 B_2(x)f''(x)\,dx$. Of course, we can insert the value $B_2 = \frac{1}{6}$. Integrating by parts again, using the fact that $B_3(0) = B_3(1) = 0$, we obtain

$$\begin{aligned} R_2 &= -\tfrac{1}{6}\Big[B_3(x)f''(x)\Big]_0^1 + \tfrac{1}{6}\int_0^1 B_3(x)f^{(3)}(x)\,dx \\ &= \tfrac{1}{6}\int_0^1 B_3(x)f^{(3)}(x)\,dx. \end{aligned}$$

As before, we can transfer these expressions to $[r, r+1]$ by considering $f(x+r)$, with $B_k(x)$ replaced by $\tilde{B}_k(x) = B_k(x - [x])$. We then combine over these intervals for $m \le r \le n-1$ to obtain

$$S^*_{m,n}(f) - I_{m,n}(f) = \tfrac{1}{2}B_2\Big(f'(n) - f'(m)\Big) + R_2(m,n),$$

where (for example) $R_2(m,n) = -\frac{1}{2}\int_m^n \tilde{B}_2(x)f''(x)\,dx$.

To express the result that emerges when the process is repeated, we write

$$E_{2k}(n) =: \sum_{j=1}^{k} \frac{B_{2j}}{(2j)!} f^{(2j-1)}(n), \tag{30}$$

also $E_0(n) = 0$. (Warning: this notation is not standard!) In particular,

$$E_2(n) = \tfrac{1}{2}B_2 f'(n) = \tfrac{1}{12}f'(n),$$

$$E_4(n) = \frac{B_2}{2}f'(n) + \frac{B_4}{4!}f^{(3)}(n) = \tfrac{1}{12}f'(n) - \tfrac{1}{720}f^{(3)}(n).$$

(These two cases are all that we will use in most examples.) We now state the full Euler-Maclaurin formula:

THEOREM 8. *Suppose that f has $2k+1$ derivatives on $[m,n]$, where $k \ge 1$. Then*

$$S^*_{m,n}(f) - I_{m,n}(f) = E_{2k}(n) - E_{2k}(m) + R_{2k}(m,n), \tag{31}$$

where

$$R_{2k}(m,n) = -\frac{1}{(2k)!}\int_m^n \tilde{B}_{2k}(x)f^{(2k)}(x)\,dx \tag{32}$$

$$= \frac{1}{(2k+1)!}\int_m^n \tilde{B}_{2k+1}(x)f^{(2k+1)}(x)\,dx. \tag{33}$$

Proof. Again, we prove the statements for the interval $[0,1]$, then transfer them to $r, r+1]$ and combine for $m \le r \le n-1$.

The case $k = 1$ has just been discussed. Working on the interval $[0,1]$, assume (31) and (32) for a general k. Write R_{2k} for $R_{2k}(0,1)$. Then, since $B_{2k+1}(0) = B_{2k+1}(1) = 0$,

$$\begin{aligned} R_{2k} &= -\frac{1}{(2k+1)!}\Big[B_{2k+1}(x)f^{(2k)}(x)\Big]_0^1 + \frac{1}{(2k+1)!}\int_0^1 B_{2k+1}(x)f^{(2k+1)}(x)\,dx \\ &= \frac{1}{(2k+1)!}\int_0^1 B_{2k+1}(x)f^{(2k+1)}(x)\,dx, \end{aligned}$$

which is (33) for k. Integrating again, we have

$$\begin{aligned} R_{2k} &= \frac{1}{(2k+2)!}\Big[B_{2k+2}(x)f^{(2k+1)}(x)\Big]_0^1 + R_{2k+2} \\ &= \frac{1}{(2k+2)!}B_{2k+2}\Big(f^{(2k+1)}(1) - f^{(2k+1)}(0)\Big) + R_{2k+2}, \end{aligned} \tag{34}$$

where

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

Added to $E_{2k}(1) - E_{2k}(0)$, the first term gives $E_{2k+2}(1) - E_{2k+2}(0)$. Hence (31) and (32) apply for $k+1$. □

Of course, to replace $S^*_{m,n}(f)$ by $S_{m,n}(f)$, we simply add $\frac{1}{2}f(n) + \frac{1}{2}f(m)$.

We clarify the case $k = 0$: $R_0(m,n)$ equals $S^*_{m,n}(f) - I_{m,n}(f)$ itself. Formula (32) does not apply, but (33) reproduces (11).

We formulate the extension to the case where n is replaced by ∞.

COROLLARY 8.1. *Suppose, for a certain $k \ge 1$, that $f^{(r)}(x) \to 0$ as $x \to \infty$ for $1 \le r \le 2k+1$ and $\int_1^\infty |f^{(2k)}(x)|\,dx$ is convergent. Then*

$$\lim_{n\to\infty}\Big(S^*_{m,n}(f) - I_{m,n}(f)\Big) = -E_{2k}(m) + R_{2k}(m,\infty), \tag{35}$$

where $R_{2k}(m,\infty)$ is given by (32) and (33) with n replaced by ∞. □

Proof. Let $n \to \infty$ in (31). The conditions ensure that $E_{2k}(n) \to 0$ as $n \to \infty$, and that $\int_m^\infty \tilde{B}_{2k}(x)f^{(2k)}(x)\,dx$ converges. Hence we can also allow n to tend to infinity in (33). Strictly, a further observation is needed here. Denote the integrand in (33) by $u_k(x)$. Since $\lim_{x\to\infty} u_k(x) = 0$, it is correct to identify $\lim_{n\to\infty}\int_m^n u_k(x)\,dx$ with $\int_m^\infty u_k(x)\,dx$. □

Note. If $f^{(2k)}(x)$ is of one sign for large enough x, then convergence of the required integral already follows from the fact that $f^{(2k-1)}(x) \to 0$ as $x \to \infty$.

Recall from (12) that the limit in (35) equates to $\int_m^\infty \tilde{B}_1(x) f'(x)\, dx$. Of course, if $S(f)$ and $I(f)$ are convergent, then it is simply $S^*_{m,\infty}(f) - I_{m,\infty}(f)$.

When $S(f)$ and $I(f)$ diverge, Corollary 8.1 ensures the convergence of $S^*_n(f) - I_n(f)$ to an Euler-type constant L^*. Fed into (16), with $L = L^* + \frac{1}{2}f(1)$, identity (35) gives

$$S_n(f) = I_n(f) + L + \tfrac{1}{2}f(n) + E_{2k}(n) - R_{2k}(n, \infty). \tag{36}$$

It is tempting to suppose that the expressions $E_{2k}(n)$ represent the partial sums of a convergent series, but in fact this is deceptive, because of the growth of the Bernoulli numbers. Recall that $|B_{2k}| \sim 2(2k)!/(2\pi)^{2k}$. As an example, if $f(x) = 1/x$, we have $f^{(2k-1)}(n) = -(2k-1)!/n^{2k}$, so

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

which tends to infinity as $k \to \infty$. This is an *asymptotic* series, not a convergent one.

Inequalities

Since $|\tilde{B}_{2k}(x)| \le |B_{2k}|$, a simple-minded bound for $R_{2k}(m, n)$ is

$$|R_{2k}(m, n)| \le \frac{|B_{2k}|}{(2k)!} \int_m^n |f^{(2k)}(x)|\, dx.$$

In the complex case, this is the natural bound to use. However, a much neater and more useful estimation is available under a condition that is often satisfied by real functions:

THEOREM 9. *Suppose that $f^{(2k+2)}(x) \ge 0$ on $[m, n]$. If k is even, then $R_{2k}(m, n) \ge 0$, so*

$$S^*_{m,n}(f) - I_{m,n}(f) \ge E_{2k}(n) - E_{2k}(m). \tag{37}$$

Reverse inequalities hold if k is odd.

Proof. It is, of course, sufficient to prove this on the interval $[0, 1]$. Revisit the expression (34) for R_{2k} obtained in the proof of Theorem 8. It can be rewritten as

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

By Proposition 5, if k is even, then $B_{2k+2} - B_{2k+2}(x) \ge 0$ on $[0, 1]$. Since $f^{(2k+2)}(x) \ge 0$, it follows that $R_{2k} \ge 0$. The opposite inequality holds for odd k. □

Note 1. The even and odd cases can be combined by stating $(-1)^k R_{2k}(m,n) \geq 0$.

Note 2. The case $k=0$ says that if $f''(x) \geq 0$, then $S^*_{m,n}(f) \geq I_{m,n}(f)$: this is the convexity result that we saw in Proposition 3. Furthermore, the proof of Theorem 9 is an extension of the method of Proposition 3, since the $x - x^2$ appearing there equates to $B_2 - B_2(x)$.

Of course, the real force of Theorem 9 applies when $f^{(2k)}(x) \geq 0$ for all $k \geq 1$: then the partial sums $E_{2k}(n) - E_{2k}(m)$ are alternately upper and lower bounds for $S^*_{m,n}(f) - I_{m,n}(f)$.

We actually introduce a slightly stronger condition. We say that a real-valued function f is *completely monotonic* on $[m,n]$ if

$$\text{(CM)} \quad (-1)^k f^{(k)}(x) \geq 0 \text{ for all } k \geq 0 \text{ and } m \leq x \leq n.$$

In other words, $f^{(2k)}(x) \geq 0$ and $f^{(2k+1)}(x) \leq 0$ for all $k \geq 0$. Of course, it follows that the even-numbered derivatives are decreasing and the odd-numbered derivatives increasing. Also, by an easy application of the mean-value theorem, if f is completely monotonic on $[m,\infty)$ for some m, then $\lim_{x\to\infty} f^{(k)}(x) = 0$ for all $k \geq 1$. This fact, together with $\lim_{x\to\infty} f(x) = 0$, ensures the conditions needed for (35) and (36), and both statements are transformed into inequalities by $(-1)^k R_{2k}(m,\infty) \geq 0$.

We also say that f satisfies condition (CM$_k$) if (CM) holds as far as the derivative $f^{(k)}$.

The prototype examples of completely monotonic functions are $1/x^p$ for $p > 0$. Another example is e^{-ax} for $a > 0$. Also, if f is completely monotonic on $[1,\infty)$, then so are $f(x+a)$ and $f(x) - f(x+a)$ for $a > 0$.

We spell out explicitly what Theorem 9 says for $k = 0$, 1, 2. Depending on the level of accuracy wanted, one or other of these versions are what we will use in most applications.

As mentioned above, the case $k = 0$ says that if $f''(x) \geq 0$, then $S^*_{m,n}(f) - I_{m,n}(f) \geq 0$ (this equates to $R_0(m,n)$). We remark that when applied to (36), this gives

$$S_n(f) \geq I_n(f) + L + \tfrac{1}{2} f(n).$$

The cases $k = 0$ and $k = 1$ together say that for f satisfying (CM$_4$) on $[m,n]$,

$$0 \leq S^*_{m,n}(f) - I_{m,n}(f) \leq \tfrac{1}{12}[f'(n) - f'(m)]. \tag{38}$$

For some applications, this may already be strong enough. However, we now formulate the pair of inequalities combining the cases $k = 1$ and $k = 2$ (for which, of course, we need f to satisfy (CM_6)):

$$S^*_{m,n}(f) - I_{m,n}(f) = \tfrac{1}{12}[f'(n) - f'(m)] - r_{m,n}, \tag{39}$$

where

$$0 \le r_{m,n} \le \tfrac{1}{720}[f^{(3)}(n) - f^{(3)}(m)]. \tag{40}$$

(Here we have written $r_{m,n}$ for $-R_2(m,n)$.) For f satisfying (CM_6) on $[m,\infty)$, (35) and (36) become:

$$S^*_{n,\infty}(f) = I_{n,\infty}(f) - \tfrac{1}{12}f'(n) - r_n \tag{41}$$

and

$$S_n(f) = I_n(f) + L + \tfrac{1}{2}f(n) + \tfrac{1}{12}f'(n) + r_n, \tag{42}$$

where (in both cases)

$$0 \le r_n \le -\tfrac{1}{720}f^{(3)}(n). \tag{43}$$

Applications to harmonic and zeta sums

Example 1: the tail of the series for $\zeta(2)$. Let $f(x) = 1/x^2$. Then $I_{n,\infty}(f) = \frac{1}{n}$, also $f'(x) = -2/x^3$ and $f^{(3)}(x) = -24/x^5$. So by (41),

$$S^*_{n,\infty}(f) = \frac{1}{n} + \frac{1}{6n^3} - r_n, \tag{44}$$

where $0 \le r_n \le 1/(30n^5)$. Compare the earlier estimates (6) and (25). If we add ten terms and apply (44) with $n = 10$, we obtain upper and lower bounds for $\zeta(2)$ differing by less than $1/(3 \times 10^6)$.

Example 2: An inequality for $\zeta(p)$. Recall the bounds from (5) and (17): $\frac{1}{p-1} + \frac{1}{2} \le \zeta(p) \le \frac{1}{p-1} + 1$. Now apply (41), with $n = 1$ and $f(x) = 1/x^p$, where $p > 1$. Then $I_{1,\infty}(f) = \frac{1}{p-1}$, also $f'(1) = -p$ and $f^{(3)}(1) = -p(p+1)(p+2)$. So we obtain

$$\zeta(p) = \frac{1}{p-1} + \frac{1}{2} + \frac{p}{12} - r_1(p), \tag{45}$$

where

$$0 \le r_1(p) \le \tfrac{1}{720}p(p+1)(p+2).$$

These bounds are much stronger, but only for small values of p. In fact, (45) applies equally for $0 < p < 1$, since the $\rho_1(s)$ in (17) equates to $\int_1^\infty \tilde{B}_1(x)f'(x)\,dx$, which is exactly the quantity considered in Theorem 8 and its variants. (At $p = 1$, the inequality applies to $\lim_{p\to 1}(\zeta(p) - \frac{1}{p-1})$; we saw in (19) that this equals γ.)

We leave it to the sufficiently determined reader to write out an estimation of the tail of the series for $\zeta(p)$, as in Example 1.

Example 3: H_n and Euler's constant. With $f(x) = 1/x$, we have $I_n(f) = \log n$, also $f'(x) = -1/x^2$ and $f^{(3)}(x) = -6/x^4$. So (42) gives

$$H_n = \log n + \gamma + \frac{1}{2n} - \frac{1}{12n^2} + r_n, \tag{46}$$

where

$$0 \le r_n \le \frac{1}{120n^4}.$$

Regarding γ as known, we can apply (46) to evaluate H_n: for example, it gives $H_{100} = 5.18737752$ to eight d.p. (note that the term r_n is less than 10^{-10}). Viewed the other way round, we can use (46) to give bounds for γ. With $n = 10$, these bounds are are 0.57721566 and 0.57721649 (compare the actual value 0.5772156650...).

The reader can check that the next term is $-1/252n^6$. Euler-Maclaurin summation was used by Euler himself to calculate the first 15 digits of γ. In 1962, Knuth used it to compute 1271 digits. For a survey of later developments in the computation of γ, see [GS].

Example 4. Let $L_n = \sum_{r=n+1}^{2n} \frac{1}{r}$. With $f(x) = 1/x$, we have

$$L_n = S^*_{n,2n}(f) - \frac{1}{2n} + \frac{1}{4n} = S^*_{n,2n}(f) - \frac{1}{4n}.$$

Now $I_{n,2n}(f) = \log 2$, so by (39),

$$S^*_{n,2n}(f) = \log 2 + \frac{1}{12}\left(\frac{1}{n^2} - \frac{1}{(2n)^2}\right) - r_n = \log 2 + \frac{1}{16n^2} - r_n, \tag{47}$$

where

$$0 \le r_n \le \frac{1}{120}\left(\frac{1}{n^4} - \frac{1}{(2n)^4}\right) = \frac{1}{128n^4}.$$

Taking $\log 2$ as known, this gives $L_{100} = 0.6906534$ to seven d.p. Alternatively, we can apply (47) to find bounds for $\log 2$: with n taken to be only 4, these bounds are 0.693117 and 0.693148 (the true value is 0.69314718...).

Example 5. Let $U_n = \sum_{r=1}^{n} \frac{1}{2r-1}$. We derive an estimate for U_n from Examples 3 and 4. Note that

$$L_n = H_{2n} - H_n = H_{2n} - 2\left(\frac{1}{2} + \frac{1}{4} + \cdots + \frac{1}{2n}\right) = 1 - \frac{1}{2} + \frac{1}{3} - \cdots - \frac{1}{2n},$$

and hence $U_n = \frac{1}{2}(H_{2n} + L_n)$. Combining (46) (for $2n$) and (47), we obtain, after simplification

$$U_n = \tfrac{1}{2}\log n + \log 2 + \tfrac{1}{2}\gamma + \frac{1}{48n^2} + q_n, \tag{48}$$

where

$$-\frac{1}{256n^4} \le q_n \le \frac{1}{3840n^4}.$$

(It is also true $U_n = H_{2n} - \frac{1}{2}H_n$, but this gives weaker bounds for q_n.)

An alternating series

A typical alternating series can be expressed in the form $\sum_{n=1}^{\infty} f(n)$ by combining terms in pairs, as in the following example.

Example 6. Catalan's constant G is defined by

$$G = 1 - \frac{1}{3^2} + \frac{1}{5^2} - \cdots .$$

We can write it as $\sum_{n=0}^{\infty} f(n)$, where

$$f(x) = \frac{1}{(4x+1)^2} - \frac{1}{(4x+3)^2}.$$

Clearly, f is completely monotonic. We have

$$I_{n,\infty}(f) = \frac{1}{4(4n+1)} - \frac{1}{4(4n+3)} = \frac{1}{2(4n+1)(4n+3)}.$$

We limit ourselves to the weaker estimation derived from (38):

$$S^*_{n,\infty}(f) = \frac{1}{2(4n+1)(4n+3)} + r_n,$$

where

$$0 \le r_n \le \frac{2}{3}\left(\frac{1}{(4n+1)^3} - \frac{1}{(4n+3)^3}\right).$$

Using the mean-value theorem, we can state the slightly simpler bound $r_n \le 1/(64n^4)$.

Stirling's formula and other integer products

Example 7: Stirling's formula for integers. The elementary statement of Stirling's formula for integers is

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

where $C = (2\pi)^{1/2}$. Restated in logarithmic form, this is equivalent to

$$\log n! = (n + \tfrac{1}{2}) \log n - n + c + R_n,$$

where $c = \frac{1}{2}\log(2\pi)$ and $R_n \to 0$ as $n \to \infty$.

We record the estimation delivered by Euler-Maclaurin summation, at the level of accuracy of (39). We will not concern ourselves with the evaluation of c. This can be achieved using the Wallis product, and can be seen in many books, for example, [AAR, p. 20]).

Since $\log n! = S_n(f)$, where $f(x) = \log x$, the method applies naturally to the logarithmic form. However, the odd-numbered derivatives are now positive and the even-numbered ones negative, so the inequality in Theorem 9 reverses.

Now $f'(x) = 1/x$ and $f^{(3)}(x) = 2/x^3$. (Note that $\int_1^\infty f'(x)\,dx$ is divergent, but $\int_1^\infty |f''(x)|\,dx$ is convergent.) Also, $I_n(f) = n\log n - n + 1$. So there is a constant L as in (42). Writing $c = L + 1$ and reversing (43), we obtain

$$\log n! = (n + \tfrac{1}{2})\log n - n + c + \frac{1}{12n} - r_n, \tag{49}$$

where

$$0 \le r_n \le \frac{1}{360n^3}.$$

As a numerical illustration, $10! = 3,628,800$. The approximation given by $Cn^{n+1/2}e^{-n}$ is 3,598,696. The bounds given by (49), to the nearest integer, are 3,628,800 itself and 3,628,810.

We give another example on integer products.

Example 8. Let $A_n = 1.3.\ldots(2n-1)$. Then

$$A_n = \frac{(2n)!}{2.4.\ldots(2n)} = \frac{(2n)!}{2^n n!} = \frac{B_n}{2^n},$$

where $B_n = (n+1)(n+2)\ldots(2n)$. We give an estimate for $\log B_n$, and hence for $\log A_n$. Now $\log B_n = S_{n+1,2n}(f)$, where $f(x) = \log x$. Also,

$$S_{n+1,2n}(f) = S^*_{n,2n}(f) + \tfrac{1}{2}\log 2n - \tfrac{1}{2}\log n = S^*_{n,2n}(f) + \tfrac{1}{2}\log 2.$$

Further,

$$I_{n,2n}(f) = 2n\log 2n - 2n - n\log n + n = n\log n + 2n\log 2 - n.$$

Apply (39), with (40) reversed. Since $f'(2n) - f'(n) = \frac{1}{2n} - \frac{1}{n} = -\frac{1}{2n}$, we obtain

$$S^*_{n,2n} - I_{n,2n} = -\frac{1}{24n} + r_n,$$

where

$$0 \le r_n \le \frac{1}{360}\left(\frac{1}{n^3} - \frac{1}{8n^3}\right) = \frac{7}{2880n^3}.$$

Hence

$$\log B_n = n\log n + (2n + \tfrac{1}{2})\log 2 - n - \frac{1}{24n} + r_n, \tag{50}$$

and $\log A_n = \log B_n - n\log 2$.

Example 9: Stirling's formula for the gamma function. For readers with the right background, we now derive the following estimation for the gamma function, extending (49):

$$\log \Gamma(x) = (x - \tfrac{1}{2}) \log x - x + c + \frac{1}{12x} - r(x), \tag{51}$$

where $0 \le r(x) \le (1/360x^3)$. This method was given in [Jam1].

Write, as usual, $\psi(t) = \Gamma'(t)/\Gamma(t)$. We prove:

$$\psi(t) = \log t - \frac{1}{2t} - \frac{1}{12t^2} + q(t), \tag{52}$$

where $0 \le q(t) \le 1/(120t^4)$. We then deduce (51) as follows. Let

$$g(x) = \log \Gamma(x) - (x - \tfrac{1}{2}) \log x + x - \frac{1}{12x}.$$

Then

$$g'(x) = \psi(x) - \log x + \frac{1}{2x} + \frac{1}{12x^2} = q(x).$$

Now $\int_1^\infty q(t)\, dt$ converges, say to I, and

$$g(x) - g(1) = \int_1^x q(t)\, dt = I - r(x),$$

where $r(x) = \int_x^\infty q(t)\, dt \le 1/(360x^3)$.

From Euler's limit expression for the gamma function, one has $\psi(t) = \lim_{n\to\infty} \psi_n(t)$, where

$$\psi_n(t) = \log n - \sum_{r=0}^{n-1} \frac{1}{r+t}.$$

Write

$$S_n^*(t) = \frac{1}{2t} + \sum_{r=1}^{n-1} \frac{1}{r+t} + \frac{1}{2(n+t)}.$$

Clearly, $\psi(t) = \lim_{n\to\infty} \psi_n^*(t)$, where $\psi_n^*(t) = \log n - S_n^*(t) - \frac{1}{2t}$. By (39), with $f(x) = 1/(x+t)$ and $m = 0$, we have

$$S_n^*(t) = \log(n+t) - \log t + \frac{1}{12t^2} - \frac{1}{12(n+t)^2} - q_n(t),$$

where $0 \le q_n(t) \le 1/(120t^4)$. Now $\log(n+t) - \log n \to 0$ as $n \to \infty$. Taking limits as $n \to \infty$, we obtain (52), with $q(t) = \lim_{n\to\infty} q_n(t)$.

Sums of terms the form $(\log n)/n^p$

Example 10: Stieltjes constants. For integers $m \ge 1$, the Euler-type constant for the function $f(x) = (\log x)^m/x$ is called the *Stieltjes constant* γ_m. Here we just consider the case $m = 1$. The first four derivatives are

$$f'(x) = \frac{1}{x^2}(1 - \log x), \qquad f''(x) = \frac{1}{x^3}(2\log x - 3),$$

$$f^{(3)}(x) = \frac{1}{x^4}(11 - 6\log x), \qquad f^{(4)}(x) = \frac{1}{x^5}(24\log x - 50).$$

Unlike our previous examples, $(-1)^k f^{(k)}(x)$ is negative up to a certain value a_k, then positive (actually, one can check that $\log a_k = H_k$, so $f(x)$ is not completely monotonic on any interval). In particular, $f(x)$ satisfies (CM$_4$) when $\log x > \frac{25}{12}$, (so certainly for $x \geq 9$). Note that $I_n(f) = \frac{1}{2}(\log n)^2$. Using only the case $k = 1$ in (36), we deduce, for $n \geq 9$,

$$S_n(f) = \tfrac{1}{2}(\log n)^2 + \gamma_1 + \frac{\log n}{2n} - r_n,$$

where

$$0 \leq r_n \leq \frac{\log n - 1}{12n^2}.$$

With $n = 10$, this gives bounds -0.0728 and -0.0739. Taking the value $\gamma_1 \approx -0.072816$ as known, we obtain $S_{100}(f) = 10.553976$ to six d.p.

Example 11: The inequality $-\zeta'(p) < 1/(p-1)^2$

Write $S(p) = \sum_{n=1}^{\infty} (\log n)/n^p$, where $p > 1$. Note that $S(p) = -\zeta'(p)$. In the notation of these notes, $S(p) = S(f_p)$, where $f_p(x) = (\log x)/x^p$. We have $I(f_p) = 1/(p-1)^2$. We will show that $S(p) < 1/(p-1)^2$.

For $p \geq 3$, this is quite elementary. Note that

$$f_p'(x) = \frac{1}{x^{p+1}}(1 - p\log x),$$

so $f_p(x)$ is strictly decreasing when $\log x \geq 1/p$, hence for all $x \geq 2$ when $p \geq 2$. By (4), $\sum_{n=3}^{\infty} f_p(n) \leq I_{2,\infty}(f_p)$. Since $f_p(1) = 0$, our statement follows if we can show that $f_p(2) < \int_1^2 f_p(x)\,dx$. Since $\log x$ is concave, $\log x \geq (x-1)\log 2$ for $1 \leq x \leq 2$. With this inserted, we find, after simplification, that the required statement equates to $2^p \geq p^2 - p + 2$. It is easily shown that this holds for $p \geq 3$ (with equality when $p = 3$).

For $1 < p \leq 3$, we use the case $k = 1$ in Theorem 8 (note that this was proved, quite simply, ahead of the general theorem). Stated for the interval $[1, \infty)$, it says

$$S(p) - \frac{1}{(p-1)^2} = S^*(f_p) - I(f_p) = -\tfrac{1}{12}f_p'(1) + R_2 = -\tfrac{1}{12} + R_2,$$

where

$$R_2 = \tfrac{1}{6}\int_1^{\infty} \tilde{B}_3(x) f_p^{(3)}(x)\,dx.$$

Unlike all our previous examples, we now estimate $|R_2|$ using a bound for $|\tilde{B}_3(x)|$ and actual evaluation of $\int_1^{\infty} |f_p^{(3)}(x)|\,dx$. Now $B_3'(x) = 3x^2 - 3x + \frac{1}{2}$, and we find the maximum value of $|B_3(x)|$ on $[0,1]$ is $\frac{1}{12\sqrt{3}} < \frac{1}{20}$, hence

$$|R_2| < \frac{1}{120} \int_1^\infty |f_p^{(3)}(x)|\, dx.$$

Now

$$f_p''(x) = \frac{1}{x^{p+2}} \Big(p(p+1)\log x - (2p+1) \Big),$$

$$f_p^{(3)}(x) = \frac{1}{x^{p+3}} \Big((3p^2+6p+2) - p(p+1)(p+2)\log x \Big).$$

So $f_p^{(3)}(x)$ is positive on $[1, x_0)$ and negative on (x_0, ∞), where

$$\log x_0 = \frac{3p^2+6p+2}{p(p+1)(p+2)} = \frac{3}{p+1} + \frac{2}{p(p+1)(p+2)}.$$

Denote this expression by $h(p)$. Clearly, $h(p)$ decreases with p. Also, $h(3) = \frac{47}{60} > \log 2$, so $x_0 > 2$ when $1 < p \le 3$. So we have

$$\int_1^\infty |f_p^{(3)}(x)|\, dx = \int_1^{x_0} f_p^{(3)}(x)\ dx - \int_{x_0}^\infty f_p^{(3)}(x)\ dx = 2f_p''(x_0) - f_p''(1).$$

Now $-f_p''(1) = 2p+1 \le 7$ for $1 < p \le 3$. Also,

$$f_p''(x_0) = \frac{1}{x_0^{p+2}} \left(\frac{3p^2+6p+2}{p+2} - (2p+1) \right) = \frac{p(p+1)}{(p+2)x_0^{p+2}} < \frac{p}{2^{p+2}} < \frac{1}{4}.$$

Hence $\int_1^\infty |f_p^{(3)}(x)|\, dx < 8$, so $|R_2| < \frac{1}{15}$, and finally, for $1 < p \le 3$,

$$S(p) < \frac{1}{(p-1)^2} - \frac{1}{12} + \frac{1}{15} = \frac{1}{(p-1)^2} - \frac{1}{60}.$$

Of course, a sharper estimate can be given with a little more effort.

Recall that $\zeta(p) - \frac{1}{p-1} \to \gamma$ as $p \to 1^+$. In the same way, we see that $S(p) - 1/(p-1)^2 \to \gamma_1$ as $p \to 1^+$.

Remark. For a particular p, we can apply our previous methods for numerical approximation to $S(p)$. For $p = 2$, after only adding four terms, one obtains the value $S(2) = 0.93755$ to five decimal places.

Further extension of the zeta function

Theorem 8 can be used to extend $\zeta(s)$ to the whole complex plane. Let $f(x) = 1/x^s$. By Corollary 8.1, with $m = 1$, we have, for $\sigma > 1$,

$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} - E_{2k}(1) + R_{2k}(1, \infty, s), \tag{53}$$

where $E_{2k}(n)$ is defined by (30) and $R_{2k}(1,\infty,s)$ is given by (33). Now $f^{(2k+1)}(x) = c_{2k+1}/x^{s+2k+1}$ for a certain coefficient c_{2k+1}, and

$$\int_1^\infty \frac{1}{x^\sigma + 2k + 1}\,dx$$

is convergent when $\sigma > -2k$. Also, $\tilde{B}_{2k+1}(x)$ is bounded, so the integral defining $R_{2k}(1,\infty,s)$ converges for such s, and we take (53) as the definition of $\zeta(s)$ for such s. When the process is repeated with $2k+2$ instead of $2k$, consistency requires

$$-E_{2k}(1) + R_{2k}(1,\infty,s) = -E_{2k+2}(1) + R_{2k+2}(1,\infty,s)$$

when $\sigma > -2k$. This is ensured by (35), since both equate to the limit on the left-hand side.

This defines $\zeta(s)$ step by step on the whole complex plane. There are other, arguably better, methods that achieve it in one step. One rather attractive method [St, chap. 8] uses the Bernoulli numbers. For other methods see [Ap, chap. 12]. By the principle of analytic continuation, all such methods are equivalent, provided that they define a holomorphic function.

However, the Euler-Maclaurin approach is just what is needed for computing values. For this purpose, we proceed exactly as we did for (20) to derive the following expression incorporating partial sums of the original series:

$$\zeta(s) = \sum_{r=1}^{n-1} \frac{1}{r^s} + \frac{1}{2n^s} + \frac{n^{1-s}}{s-1} - E_{2k}(n) + R_{2k}(n,\infty,s). \tag{54}$$

We have kept this looking reasonably simple by adhering to our notation $E_{2k}(n)$: if its definition is substituted, and the derivatives written out, it looks seriously complicated! For some worked examples, see [Edw, chap. 6].

Sums of integer powers

Let $S(p,n) = \sum_{r=1}^n r^p$, where p is a positive integer. Euler-Maclaurin summation delivers at once the well-known closed expression for $S(p,n)$ in terms of the Bernoulli numbers (though it should be said that a direct proof is not hard). We rewrite $S(p,n)$ as $\sum_{r=0}^n r^p$, so, in our standing notation $S(p,n) = S_{0,n}(f)$, where $f(x) = x^p$. Also, for this purpose, it is helpful to rewrite the definition (11) of $E_{2k}(n)$ to include the odd terms, although in fact they are zero:

$$E_k(n) = \sum_{j=2}^k \frac{B_j}{j!} f^{(j-1)}(n).$$

By Theorem 8, applied to $2k$ and $2k+1$, we see that if $f^{(k)}(x) = 0$ for all x, then $S^*_{0,n}(f) - I_{0,n}(f) = E_k(n) - E_k(0)$: the remainder term is zero. For $f(x) = x^p$, we have $f^{(j)}(0) = 0$ for

$j \le p-1$ and $f^{(p)}(n) = f^{(p)}(0) = p!$. Now taking $k = p+1$ and adding the term $\frac{1}{2}n^p$, we conclude:

$$S(p,n) = \frac{n^{p+1}}{p+1} + \tfrac{1}{2}n^p + \sum_{j=2}^{p} \frac{B_j}{j!} p(p-1)\dots(p-j+2)n^{p-j+1}. \tag{55}$$

Equivalently,

$$(p+1)S(p,n) = n^{p+1} + \tfrac{1}{2}(p+1)n^p + \sum_{j=2}^{p} B_j \binom{p+1}{j} n^{p-j+1}. \qquad \square \tag{56}$$

There are further ways to rewrite this formula. To obtain $S(p,n-1)$ instead of $S(p,n)$, subtract n^p in (55). The second term becomes $-\frac{1}{2}n^p = B_1 n^p$. Since also $B_0 = 1$, we can restate (56) as

$$(p+1)S(p,n-1) = \sum_{j=0}^{p} B_j \binom{p+1}{j} n^{p-j+1}.$$

A variant based on mid-points

Instead of the trapezium rule, it is equally natural to compare $f(r)$ with $K_r(f)$, where

$$K_r(f) = \int_{r-1/2}^{r+1/2} f(x)\,dx.$$

When added, this will lead to direct estimations of $S_{m,n}(f)$, without having to halve the end values. Note that $f(r)$ is the mid-point estimate for the integral $K_r(f)$, and will underestimate it when f is convex. This variant of Euler-Maclaurin summation was described by De Temple and Wang [DTW], though only presented for the particular case of the harmonic series. I do not know if there are earlier references for it.

The starting point is the following analogue of Proposition 1, which we state on the interval $[-\frac{1}{2}, \frac{1}{2}]$ (do not be alarmed by the negative values of x: the result will be applied to $f(x+r)$ as before).

PROPOSITION 10. *With this notation, we have*

$$\begin{aligned} f(0) - K_0(f) &= \int_0^{1/2} (x - \tfrac{1}{2})\Big(f'(x) - f'(-x)\Big)\,dx. && (57)\\ &= \int_{-1/2}^{1/2} \tilde{B}_1(x) f'(x)\,dx. && (58) \end{aligned}$$

Proof. Write $g(x) = f(x) + f(-x)$, so that $g'(x) = f'(x) - f'(-x)$. Note that $\int_0^{1/2} f(-x)\,dx = \int_{-1/2}^{0} f(x)\,dx$, so that $\int_0^{1/2} g(x)\,dx = \int_{-1/2}^{1/2} f(x)\,dx = K_0(f)$. Integrate by parts:

$$\begin{aligned}
\int_0^{1/2} (x - \tfrac{1}{2}) g'(x)\, dx &= \Big[(x - \tfrac{1}{2}) g(x)\Big]_0^{1/2} - \int_0^{1/2} g(x)\, dx \\
&= \tfrac{1}{2} g(0) - K_0(f) \\
&= f(0) - K_0(f).
\end{aligned}$$

Further,

$$-\int_0^{1/2} (x - \tfrac{1}{2}) f'(-x)\, dx = \int_{-1/2}^{0} (y + \tfrac{1}{2}) f'(y)\, dy,$$

and for $-\frac{1}{2} \le y < 0$, we have $[y] = -1$, so $y + \frac{1}{2} = y - [y] - \frac{1}{2} = \tilde{B}_1(y)$, hence (58). $\square$

Transferring to $[r - \frac{1}{2}, r + \frac{1}{2})$ and combining, we deduce as before:

COROLLARY 10.1. *We have*

$$S_{m,n}(f) - \int_{m-1/2}^{n+1/2} f(x)\, dx = \int_{m-1/2}^{n+1/2} \tilde{B}_1(x) f'(x)\, dx. \qquad \square \tag{59}$$

It is clear from (57) (more easily than (58)) that if $f'(x)$ is increasing (so f is convex), then $f(r) \le K_r(f)$, as mentioned above.

We now state the result obtained by repeated integration by parts, corresponding to Theorem 8. For now, we present it in the form derived from (57) rather than (58). Define

$$F_{2k}(x) = \sum_{j=1}^{k} \frac{B_{2j}(\frac{1}{2})}{(2j)!} f^{(2j-1)}(x). \tag{60}$$

Recall that the numbers $B_n(\frac{1}{2})$ are given by (29). In particular, inserting the values $B_2(\frac{1}{2}) = -\frac{1}{12}$ and $B_4(\frac{1}{2}) = \frac{7}{240}$, we have

$$F_2(x) = -\tfrac{1}{24} f'(x),$$

$$F_4(x) = -\tfrac{1}{24} f'(x) + \tfrac{7}{5760} f^{(3)}(x).$$

THEOREM 11. *If f has $2k+1$ derivatives on $[m - \frac{1}{2}, n + \frac{1}{2}]$, then*

$$S_{m,n}(f) - \int_{m-1/2}^{n+1/2} f(x)\, dx = F_{2k}(n + \tfrac{1}{2}) - F_{2k}(m - \tfrac{1}{2}) + T_{2k}(m,n), \tag{61}$$

in which $T_{2k}(m,n) = \sum_{r=m}^{n} \sigma_{2k,r}$, where

$$\begin{aligned}
\sigma_{2k,r} &= -\frac{1}{(2k)!} \int_0^{1/2} B_{2k}(x) \Big(f^{(2k)}(x + r) + f^{(2k)}(-x + r) \Big)\, dx & (62) \\
&= \frac{1}{(2k+1)!} \int_0^{1/2} B_{2k+1}(x) \Big(f^{(2k+1)}(x + r) - f^{(2k+1)}(-x + r) \Big)\, dx. & (63)
\end{aligned}$$

Further, if f is completely monotonic on $[m-\frac{1}{2}, n+\frac{1}{2}]$, then $(-1)^{k-1}T_{2k}(m,n) \geq 0$.

Proof. Concentrating first on the interval $[-\frac{1}{2}, \frac{1}{2}]$, we prove

$$f(0) - K_0(f) = F_{2k}(\tfrac{1}{2}) - F_{2k}(-\tfrac{1}{2}) + \sigma_{2k}, \tag{64}$$

where $\sigma_{2k} = \sigma_{2k,0}$ is given by (62) and (63). Applied to $f(x+r)$, this then gives

$$f(r) - K_r(f) = F_{2k}(r+\tfrac{1}{2}) - F_{2k}(r-\tfrac{1}{2}) + \sigma_{2k,r},$$

with $\sigma_{2k,r}$ as stated. We then combine for $m \leq r \leq n$ to obtain (61).

Continue to write $g(x) = f(x) + f(-x)$. Note that $g'(0) = 0$. Integrating by parts in (57), we obtain

$$\begin{aligned}
f(0) - K_0(f) &= \left[\tfrac{1}{2}B_2(x)g'(x)\right]_0^{1/2} - \tfrac{1}{2}\int_0^{1/2} B_2(x)g''(x)\,dx \\
&= \tfrac{1}{2}B_2(\tfrac{1}{2})g'(\tfrac{1}{2}) - \tfrac{1}{2}\int_0^{1/2} B_2(x)g''(x)\,dx.
\end{aligned}$$

This is the case $k=1$ in (64) and (62). Now assume (64) and (62) for a general k. Then, since $B_{2k+1}(0) = B_{2k+1}(\frac{1}{2}) = 0$,

$$\begin{aligned}
\sigma_{2k} &= -\frac{1}{(2k+1)!}\left[B_{2k+1}(x)g^{(2k)}(x)\right]_0^{1/2} + \frac{1}{(2k+1)!}\int_0^{1/2} B_{2k+1}(x)g^{(2k+1)}(x)\,dx \\
&= \frac{1}{(2k+1)!}\int_0^{1/2} B_{2k+1}(x)g^{(2k+1)}(x)\,dx,
\end{aligned}$$

which is (63) for k. Integrating again, we have

$$\begin{aligned}
\sigma_{2k} &= \frac{1}{(2k+2)!}\left[B_{2k+2}(x)g^{(2k+1)}(x)\right]_0^{1/2} + \sigma_{2k+2} \\
&= \frac{1}{(2k+2)!}B_{2k+2}(\tfrac{1}{2})g^{(2k+1)}(\tfrac{1}{2}) + \sigma_{2k+2},
\end{aligned}$$

where

$$\sigma_{2k+2} = -\frac{1}{(2k+2)!}\int_0^{1/2} B_{2k+2}(x)g^{(2k+2)}(x)\,dx,$$

hence (64) and (62) for $k+1$.

If f is completely monotonic, then $f^{(2k+1)}(x)$ is increasing, so $f^{(2k+1)}(r+x) \geq f^{(2k+1)}(r-x)$ for $0 \leq x < \frac{1}{2}$. Also, by Proposition 5, $(-1)^{k-1}B_{2k+1}(x) \geq 0$ for $0 \leq x \leq \frac{1}{2}$. Hence $(-1)^{k-1}\sigma_{2k,r} \geq 0$ for each r, so $(-1)^{k-1}T_{2k}(m,n) \geq 0$. □

Now considering the limit as $n \to \infty$ as in Corollary 8.1, we deduce:

COROLLARY 11.1. *Suppose, for a certain $k \geq 1$, that $f^{(r)}(x) \to 0$ as $x \to \infty$ for $1 \leq r \leq 2k+1$ and $\int_1^\infty |f^{(2k)}(x)|\,dx$ is convergent. Then*

$$\lim_{n\to\infty}\left(S_{m,n}(f) - \int_{m-1/2}^{n+1/2} f(x)\,dx\right) = -F_{2k}(m-\tfrac{1}{2}) + T_{2k}(m,\infty), \tag{65}$$

where $T_{2k}(m,\infty) = \sum_{r=m}^\infty \sigma_{2k,r}$.

Proof. The conditions ensure that $F_{2k}(n+\frac{1}{2}) \to 0$ as $n \to \infty$ and that $\sum_{r=1}^\infty \sigma_{2k,r}$ is convergent. □

When the series and integral converge, the left-hand side of (65) is simply $S_{m,\infty}(f) - \int_{m-1/2}^\infty f(x)\,dx$.

When the series and integral diverge, (65) (with $m=1$) gives

$$S_n(f) - \int_{1/2}^{n+1/2} f(x)\,dx \to L' \text{ as } n \to \infty,$$

where

$$L' = -F_{2k}(\tfrac{1}{2}) + T_{2k}(1,\infty).$$

Substituting this into (61) (also with $m=1$), and noting that $T_{2k}(1,\infty) = T_{2k}(1,n) + T_{2k}(n+1,\infty)$, we obtain

$$\begin{aligned} S_n(f) &= \int_{1/2}^{n+1/2} f(x)\,dx + L' + F_{2k}(n+\tfrac{1}{2}) - T_{2k}(n+1,\infty) & (66)\\ &= \int_{1}^{n+1/2} f(x)\,dx + L + F_{2k}(n+\tfrac{1}{2}) - T_{2k}(n+1,\infty), & (67)\end{aligned}$$

where $L = L' + \int_{1/2}^1 f(x)\,dx$. Provided that $\lim_{x\to\infty} f(x) = 0$, L equates to the Euler-type constant $\lim_{n\to\infty}[S_n(f) - I_n(f)]$.

As before, we state explicitly the inequalities for completely monotonic functions resulting from the cases $k=1$ and $k=2$. Theorem 11 becomes

$$S_{m,n}(f) - \int_{m-1/2}^{n+1/2} f(x)\,dx = -\frac{1}{24}\left(f'(n+\tfrac{1}{2}) - f'(m-\tfrac{1}{2})\right) + T_2(m,n), \tag{68}$$

where

$$0 \leq T_2(m,n) \leq \tfrac{7}{5760}\left(f^{(3)}(n+\tfrac{1}{2}) - f^{(3)}(m-\tfrac{1}{2})\right).$$

Compare (40). The factor $\frac{1}{720}$ has been replaced by the slightly smaller factor $\frac{7}{5760}$.

For the tail of a convergent series, corresponding to (41), we have

$$S_{m,\infty}(f) = \int_{m-1/2}^\infty f(x)\,dx + \tfrac{1}{24}f'(m-\tfrac{1}{2}) + s_m, \tag{69}$$

where

$$0 \le s_m \le -\tfrac{7}{5760} f^{(3)}(m - \tfrac{1}{2}). \tag{70}$$

For the $\zeta(2)$ series, this gives the following estimation, which can be compared with (44):

$$\sum_{r=m}^{\infty} \frac{1}{r^2} = \frac{1}{m - \frac{1}{2}} - \frac{1}{12(m - \frac{1}{2})^3} + s_m,$$

where

$$0 \le s_m \le \frac{7}{240(m - \frac{1}{2})^5)}.$$

When the series and integral diverge, (67) becomes

$$S_n(f) = \int_1^{n+1/2} f(x)\,dx + L - \tfrac{1}{24}(n + \tfrac{1}{2}) - t_n, \tag{71}$$

where

$$0 \le t_n \le -\frac{7}{5760} f^{(3)}(n + \tfrac{1}{2}). \tag{72}$$

In particular, for the harmonic series,

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

where

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

Compare (46). The term $1/2n$ has been absorbed into the log term, resulting (arguably) in an estimation which is at least as natural.

The expressions for $\sigma_{2k,r}$ in Theorem 11 have served quite well for these applications, but it does not look as if they join together to form a single integral as in (32). In fact, they do so, as we saw for the first stage in Proposition 10. The new feature is that $\tilde{B}_{2k}(x)$ has a discontinuity at the middle of each interval $[r - \frac{1}{2}, r + \frac{1}{2}]$.

PROPOSITION 12. *With the notation of Theorem 11, we have*

$$T_{2k}(m,n) = -\frac{1}{(2k)!} \int_{m-1/2}^{n+1/2} \tilde{B}_{2k}(x) f^{(2k)}(x)\,dx \tag{73}$$

$$= \frac{1}{(2k+1)!} \int_{m-\frac{1}{2}}^{n+1/2} \tilde{B}_{2k+1}(x) f^{(2k+1)}(x)\,dx. \tag{74}$$

Proof. Again consider the interval $[-\frac{1}{2}, \frac{1}{2}]$, so that σ_{2k} is given by (62), with $r = 0$. So $\sigma_{2k} = -1/[(2k)!](I_1 + I_2)$, where

$$I_1 = \int_0^{1/2} B_{2k}(x) f^{(2k)}(x)\,dx,$$

$$I_2 = \int_0^{1/2} B_{2k}(x) f^{(2k)}(-x)\, dx.$$

For I_1, just note that for $0 \le x \le \frac{1}{2}$, we have $\tilde{B}_2(x) = B_2(x)$. Now consider I_2. By Proposition 4, $B_{2k}(1-x) = B_{2k}(x)$ for $0 \le x \le \frac{1}{2}$, so

$$\begin{aligned} I_2 &= \int_0^{1/2} B_{2k}(1-x) f^{(2k)}(-x)\, dx \\ &= \int_{-1/2}^{0} B_{2k}(1+y) f^{(2k)}(y)\, dy. \end{aligned}$$

For $-\frac{1}{2} \le y < 0$, we have $[y] = -1$, so $B_{2k}(1+y) = B_{2k}(y - [y]) = \tilde{B}_{2k}(y)$. Now combining with I_1 again, we see that

$$\sigma_{2k} = \int_{-1/2}^{1/2} \tilde{B}_{2k}(x) f^{(2k)}(x)\, dx.$$

Applying this to $f(x+r)$ and substituting $x + r = y$, we deduce

$$\sigma_{2k,r} = \int_{r-1/2}^{r+1/2} \tilde{B}_{2k}(y) f^{(2k)}(y)\, dy.$$

Combining intervals, we obtain (73). The proof of (74) is similar, with the adjustment that $B_{2k+1}(1-x) = -B_{2k+1}(x)$. □

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