

The Euler–Maclaurin and Taylor Formulas: Twin, Elementary Derivations

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Introduction

The calculator is perfectly suited to brute force processes. Want to sum a few hundred terms of a series? The calculator can do it almost instantly. The existence of the calculator might suggest that computational leverage provided by calculus is no longer needed. But although the arena in which leverage is required has shifted a bit, our ability to compute is still immeasurably enriched by the power of calculus. Indeed, that power is used in the design of modern software and calculators. For instance, programs like *Maple* and *Mathematica* compute sums like $\sum_{k=1}^{1000^{1000}} 1/k$ and $\sum_{k=1}^{\infty} 1/k^3$ in the blink of an eye. How do they do it?

The *Mathematica* manual [18, p. 917] reveals that *Mathematica* actually uses the famous *Euler–Maclaurin* (E–M) *formula*, of which one form states that for $m \leq n$,

$$\sum_{k=m}^n f(k) - \int_m^n f(x) dx = \frac{1}{2} [f(m) + f(n)] + \frac{1}{12} [f'(n) - f'(m)] + \rho(f; m, n),$$

where

$$|\rho(f; m, n)| \leq \frac{1}{120} \int_m^n |f'''(x)| dx.$$

Let us illustrate how this formula works. By setting $f(x) = 1/x$ we get, for $m \leq n$,

$$\sum_{k=1}^n \frac{1}{k} = \left(\sum_{k=1}^{m-1} \frac{1}{k} - \ln m + \frac{1}{2m} + \frac{1}{12m^2} \right) + \left(\ln n + \frac{1}{2n} - \frac{1}{12n^2} \right) + \rho(m, n),$$

where

$$|\rho(m, n)| \leq \frac{1}{120} \left(\frac{2}{m^3} - \frac{2}{n^3} \right) < \frac{1}{60m^3}.$$

For example, $|\rho(m, n)| \leq 1.7 \times 10^{-8}$ for $n \geq m \geq 100$, so

$$\begin{aligned} \sum_{k=1}^n \frac{1}{k} &= \left(\sum_{k=1}^{99} \frac{1}{k} - \ln 100 + \frac{1}{200} + \frac{1}{120000} \right) + \left(\ln n + \frac{1}{2n} - \frac{1}{12n^2} \right) + \rho(100, n) \\ &= 0.577215664 + \ln n + \left(\frac{1}{2n} - \frac{1}{12n^2} \right) + \delta(n). \end{aligned}$$

The first expression in parentheses above was truncated to nine places; the resulting error was combined with the error $\rho(100, n)$ to give a new error $\delta(n)$, where

$$|\delta(n)| < 10^{-9} + 1.7 \times 10^{-8} = 1.8 \times 10^{-8}$$

for $n \geq 100$. For $n = 1000^{1000}$ we read

$$S := \sum_{k=1}^{1000^{1000}} \frac{1}{k} = (0.577215664 + \ln 1000^{1000}) + \delta(1000^{1000})$$

and compute the first parenthesized expression to nine places. The error of this approximation we combine with $\delta(1000^{1000})$ to get a new error Δ with $S = 6908.332494646 \dots + \Delta$. Since $|\Delta| < 1.9 \times 10^{-8}$, $S = 6908.3324946 \dots$ is correct to seven decimal places.

The E–M summation formula is among the most remarkable formulas of mathematics [15, p. 11]. In fact, neither Euler nor Maclaurin found this formula with remainder; the first to do so was Poisson, in 1823 ([14], see also [8, p. 471] or [11, p. 521]). Since then the E–M formula has been derived in different ways; one of the earliest derivations (1834) was presented by Jacobi [10]. Boas [3, p. 246] gave an elegant derivation of the E–M formula using the Stieltjes integral. An elementary derivation of this formula has long been known using the method of integration by parts (see Glaisher as cited in [4]; see also [17, pp. 125, 127]). Apostol [1] presents another nice elementary derivation of the E–M formula by the same means.

Every standard textbook in analysis contains Taylor’s formula, but few include the E–M formula, perhaps because of its somewhat cumbersome form and its relatively complicated derivation. In this paper we present a completely elementary derivation of the E–M formula, which also produces Taylor’s formula. The main idea stems from the observation that, when integrating a function whose p th derivative is more “controllable” than the function itself, we may apply the method of the integration by parts p times. If we organize this process appropriately, we obtain such interesting formulas as Taylor’s formula and the E–M formula.

Preliminaries

For an integer $n \geq 0$ and a closed interval $[a, b]$, let $C^n[a, b]$ denote the set of all n -times continuously differentiable functions defined on $[a, b]$. The *integration by parts* formula asserts that

$$\int_a^b u(t) v'(t) dt = [u(t) v(t)]_a^b - \int_a^b u'(t) v(t) dt$$

for $u, v \in C^1[a, b]$. This is easily generalized by induction to the following elementary but important lemma on *repeated* integration by parts in closed form:

Lemma. For $u, v \in C^n[a, b]$,

$$\int_a^b u(t) v^{(n)}(t) dt = \left[\sum_{i=0}^{n-1} (-1)^i u^{(i)}(t) v^{(n-1-i)}(t) \right]_a^b + (-1)^n \int_a^b u^{(n)}(t) v(t) dt.$$

Example 1. To calculate $\int x^3 e^x dx$, we substitute $a = 0$, $b = x$, $u(t) := t^3$; $v(t) := e^t$; and $n = 4$ into the preceding equation to obtain

$$\int x^3 e^x dx = \left[\sum_{i=0}^3 (-1)^i (t^3)^{(i)} (e^t)^{(3-i)} \right]_0^x + 0 + C = (x^3 - 3x^2 + 6x - 6) e^x + C.$$

If we put $a = 0$, $b = 1$, and $u, v \in C^n[0, 1]$ into the lemma above and then get rid of the factors $(-1)^i$ by replacing $v(t)$ with $v(1 - t)$, and then cancel $(-1)^n$, we arrive at the basic equality

$$\int_0^1 u(t) v^{(n)}(1 - t) dt = \sum_{i=0}^{n-1} [u^{(i)}(0) v^{(n-1-i)}(1) - u^{(i)}(1) v^{(n-1-i)}(0)] + \int_0^1 v(1 - t) u^{(n)}(t) dt. \quad (1)$$

Both Taylor's formula and the E-M formula can be derived by judicious choices of v in (1).

Taylor's formula

To obtain Taylor's formula it suffices to take for v in formula (1) a function whose derivative vanishes to an appropriate high order. Our derivation is in two steps.

Unit increment. Let p be any nonnegative integer and $u \in C^{p+1}[0, 1]$. In (1) we set $v(t) = t^p/p!$ and $n = p + 1$. Since $v^{(p+1)}(t) \equiv 0$ we have $\int_0^1 u(t)v^{(p+1)}(1 - t)dt = 0$. Since $v^{(j)}(t) \equiv t^{p-j}/(p - j)!$ for $0 \leq j \leq p$, we get from (1) the equality

$$u(0) - u(1) + \sum_{i=1}^p \left[\frac{u^{(i)}(0)}{i!} - 0 \right] + \int_0^1 \frac{(1 - t)^p}{p!} u^{(p+1)}(t) dt = 0.$$

Including $u(0)$ under the summation sign produces

$$u(1) = \sum_{i=0}^p \frac{u^{(i)}(0)}{i!} + \frac{1}{p!} \int_0^1 (1 - t)^p u^{(p+1)}(t) dt, \quad (2)$$

which is Taylor's formula for a unit increment.

Arbitrary increment. For a function $f \in C^{p+1}[a, b]$ and numbers x_0 and $x_0 + h$ in $[a, b]$, we define the function $u \in C^{p+1}[0, 1]$ by $u(t) = f(x_0 + ht)$. Since $u^{(i)}(t) \equiv h^i f^{(i)}(x_0 + ht)$ for $i = 0, 1, \dots, p + 1$, we obtain from (2)

$$f(x_0 + h) = u(1) = \sum_{i=0}^p \frac{f^{(i)}(x_0)}{i!} h^i + \frac{h^{p+1}}{p!} \int_0^1 (1 - t)^p f^{(p+1)}(x_0 + ht) dt,$$

which is *Taylor's formula of order p with remainder*.

Euler-Maclaurin formula

To obtain this formula it suffices to take for v in the identity (1) a function whose derivative of an appropriately high order is identically equal to 1.

Connecting integrals and derivatives Let p be a positive integer, $u \in C^p[0, 1]$, and v a function such that $v^{(p)}(t) \equiv 1$. Then we have $\int_0^1 u(t)dt = \int_0^1 u(t)v^{(p)}(1 - t)dt$, and the formula (1) can be applied. So, we want a sequence $\{v_k\}$ of polynomials, such that $v_k^{(k)}(t) \equiv 1$ for $k \geq 0$. An easy approach is to put

$$v_0(t) := 1 \quad \text{and} \quad v'_k(t) := v_{k-1}(t) \quad \text{for} \quad k \geq 1. \tag{3}$$

This recursion formula does not uniquely determine the sequence $\{v_k\}$, but (3) implies that $v_p^{(j)} = v_{p-j}$ for $j = 0, 1, \dots, p$, so $v_p^{(p-1-i)} = v_{i+1}$ for $i = 0, 1, \dots, p - 1$. Putting this into (1) we obtain for $n = p$ the equality

$$\int_0^1 u(t) dt = \sum_{j=1}^p [u^{(j-1)}(0) v_j(1) - u^{(j-1)}(1) v_j(0)] + \int_0^1 v_p(1-t) u^{(p)}(t) dt. \tag{4}$$

To simplify the expression in square brackets we require, in addition, that

$$v_j(0) = v_j(1) \quad \text{for} \quad j = 2, 3, \dots \tag{5a}$$

By (3), $v_j(1) - v_j(0) = \int_0^1 v'_j(t) dt = \int_0^1 v_{j-1}(t) dt$ for $j \geq 1$, so (5a) is equivalent to

$$\int_0^1 v_k(t) dt = 0 \quad \text{for} \quad k = 1, 2, 3, \dots \tag{5b}$$

The polynomial sequence (v_k) is now completely determined by (3) and (5b). For example, (3) implies $v_1(t) \equiv t + C$, and from (5b) we find $C = -1/2$, so $v_1(t) \equiv t - 1/2$. Since $v_1(0) = -1/2 = -v_1(1)$, we can rewrite (4), using (5a), in the form

$$u(1) = \int_0^1 u(t) dt + \sum_{j=1}^p v_j(1) [u^{(j-1)}(t)]_0^1 - \int_0^1 v_p(1-t) u^{(p)}(t) dt. \tag{6}$$

Connecting sums and integrals Our next goal is to connect summation with integration. To this end, let n and p be positive integers and let $\varphi \in C^p[0, n]$. We define functions u_i by $u_i(t) = \varphi(i + t)$, for $t \in [0, 1]$ and integers $i = 0, 1, \dots, n - 1$. Then $u_i \in C^p[0, 1]$ and $\sum_{i=0}^{n-1} u_i(1) = \sum_{i=1}^n \varphi(i)$. Now (6) implies the following equalities:

$$\begin{aligned} \sum_{i=1}^n \varphi(i) &= \sum_{i=0}^{n-1} \left\{ \int_0^1 u_i(t) dt + \sum_{j=1}^p v_j(1) [u_i^{(j-1)}(t)]_0^1 - \int_0^1 v_p(1-t) u_i^{(p)}(t) dt \right\} \\ &= \sum_{i=0}^{n-1} \int_i^{i+1} \varphi(\tau) d\tau + \sum_{i=0}^{n-1} \sum_{j=1}^p v_j(1) [\varphi^{(j-1)}(t)]_i^{i+1} \\ &\quad - \sum_{i=0}^{n-1} \int_0^1 v_p(1-t) \varphi^{(p)}(i+t) dt \\ &= \int_0^n \varphi(\tau) d\tau + \sum_{j=1}^p v_j(1) \sum_{i=0}^{n-1} [\varphi^{(j-1)}(t)]_i^{i+1} \\ &\quad - \sum_{i=0}^{n-1} \int_0^1 v_p(1-t) \varphi^{(p)}(i+t) dt \\ &= \int_0^n \varphi(\tau) d\tau + \sum_{j=1}^p v_j(1) [\varphi^{(j-1)}(t)]_0^n - \sum_{i=0}^{n-1} \int_0^1 v_p(1-t) \varphi^{(p)}(i+t) dt. \end{aligned}$$

Since $v_1(1) = -v_1(0) = 1/2$, and $v_j(0) = v_j(1)$ for $j \geq 2$, we can rewrite the last equality as

$$\sum_{i=0}^{n-1} \varphi(i) = \int_0^n \varphi(t) dt + \sum_{j=1}^p v_j(0) [\varphi^{(j-1)}(t)]_0^n - \sum_{i=0}^{n-1} \int_0^1 v_p(1-t) \varphi^{(p)}(i+t) dt. \quad (7)$$

In order to simplify the last sum in this formula we introduce periodic functions $w_i(x)$ ($i \geq 0$), defined by $w_i(x) := v_i(x - \lfloor x \rfloor)$ for any real x . (Here $\lfloor x \rfloor$ denotes the integer part of x .) Then

$$w_i(x) = v_i(x) \text{ for } 0 \leq x < 1 \quad \text{and} \quad w_i(x+1) = w_i(x) \text{ for } x \in \mathbb{R}. \quad (8)$$

As 1 is the period of $w_i(x)$, we have $w_i(x+m) = w_i(x)$ for $x \in \mathbb{R}$ and $m \in \mathbb{Z}$. Substituting $i+t = \tau$ in the integrals we get

$$\begin{aligned} \sum_{i=0}^{n-1} \int_0^1 v_p(1-t) \varphi^{(p)}(i+t) dt &= \sum_{i=0}^{n-1} \int_0^1 w_p(-t) \varphi^{(p)}(i+t) dt \\ &= \sum_{i=0}^{n-1} \int_i^{i+1} w_p(i-\tau) \varphi^{(p)}(\tau) d\tau \\ &= \sum_{i=0}^{n-1} \int_i^{i+1} w_p(-\tau) \varphi^{(p)}(\tau) d\tau \\ &= \int_0^n w_p(-\tau) \varphi^{(p)}(\tau) d\tau. \end{aligned}$$

Thus, from (7) we conclude

$$\sum_{i=0}^{n-1} \varphi(i) = \int_0^n \varphi(t) dt + \sum_{j=1}^p v_j(0) [\varphi^{(j-1)}(t)]_0^n - \int_0^n w_p(-t) \varphi^{(p)}(t) dt. \quad (9)$$

Connecting Riemann sums and integrals For a function $f \in C^p[a, b]$ and a positive integer n we put $h = (b-a)/n$ and define φ by $\varphi(t) := f(a+ht)$. Hence $\varphi \in C^p[0, n]$, with $\varphi^{(j)}(t) = h^j f^{(j)}(a+ht)$, for $j = 0, 1, \dots, p$, and $\sum_{i=0}^{n-1} f(a+ih) = \sum_{i=0}^{n-1} \varphi(i)$. Now (9) becomes

$$\begin{aligned} \sum_{i=0}^{n-1} f(a+ih) &= \int_0^n \varphi(t) dt + \sum_{j=1}^p v_j(0) [\varphi^{(j-1)}(t)]_0^n - \int_0^n w_p(-t) \varphi^{(p)}(t) dt \\ &= \frac{1}{h} \int_a^b f(x) dx + \sum_{j=1}^p v_j(0) h^{j-1} [f^{(j-1)}(t)]_a^{a+hn} \\ &\quad - h^{p-1} \int_a^b w_p\left(\frac{a-x}{h}\right) f^{(p)}(x) dx, \end{aligned}$$

or

$$\begin{aligned} h \sum_{i=0}^{n-1} f(a+ih) - \int_a^b f(x) dx &= \sum_{j=1}^p v_j(0) h^j [f^{(j-1)}(x)]_a^b \\ &\quad - h^p \int_a^b w_p\left(\frac{a-x}{h}\right) f^{(p)}(x) dx. \quad (10) \end{aligned}$$

This is the E–M formula in terms of the chosen functions $v_k(x)$ and $w_k(x)$.

Better known than these functions are the *Bernoulli polynomials* $B_k(x)$ and the *Bernoulli periodic functions* $P_k(x)$, related to $v_k(x)$ and $w_k(x)$ by

$$B_k(x) := k! v_k(x) \quad \text{and} \quad P_k(x) := k! w_k(x) \tag{11}$$

for $x \in \mathbb{R}$ and $k \geq 0$. According to (3), (5b), and (8), these functions are uniquely determined by the conditions

$$B_0(x) \equiv 1; \quad B'_k(x) \equiv kB_{k-1}(x); \quad \int_0^1 B_k(x) dx = 0 \tag{12}$$

for $k \geq 1$, and by

$$P_k(x) \equiv B_k(x) \quad \text{on} \quad [0, 1) \quad \text{and} \quad P_k(x + 1) \equiv P_k(x) \quad \text{on} \quad \mathbb{R} \tag{13}$$

for all $k \geq 0$.

We can derive from (12) the first eight nonconstant Bernoulli polynomials:

$$\begin{aligned} B_1(x) &= x - \frac{1}{2} \\ B_2(x) &= x^2 - x + \frac{1}{6} = -x(1-x) + \frac{1}{6} \\ B_3(x) &= x^3 - \frac{3x^2}{2} + \frac{x}{2} = -x(1-x) \left(x - \frac{1}{2}\right) \\ B_4(x) &= x^4 - 2x^3 + x^2 - \frac{1}{30} = (x-x^2)^2 - \frac{1}{30} \\ B_5(x) &= x^5 - \frac{5x^4}{2} + \frac{5x^3}{3} - \frac{x}{6} = -\left[\frac{1}{3} + x(1-x)\right] B_3(x) \\ B_6(x) &= x^6 - 3x^5 + \frac{5x^4}{2} - \frac{x^2}{2} + \frac{1}{42} = -(x-x^2)^2 \left[\frac{1}{2} + x(1-x)\right] + \frac{1}{42} \\ B_7(x) &= x^7 - \frac{7x^6}{2} + \frac{7x^5}{2} - \frac{7x^3}{6} + \frac{x}{6} = \left[\frac{1}{3} + x(1-x)(1+x(1-x))\right] B_3(x) \\ B_8(x) &= x^8 - 4x^7 + \frac{14x^6}{3} - \frac{7x^4}{3} + \frac{2x^2}{3} - \frac{1}{30} \\ &= (x-x^2)^2 \left[\frac{2}{3} + x(1-x) \left(\frac{4}{3} + x(1-x)\right)\right] - \frac{1}{30}. \end{aligned} \tag{14}$$

The numbers $B_k := B_k(0)$, $k = 0, 1, 2, \dots$ are called *Bernoulli coefficients*; from (14) we read

$$B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{6}, \quad B_3 = B_5 = B_7 = 0, \quad B_4 = B_8 = -\frac{1}{30}, \quad B_6 = \frac{1}{42}. \tag{15}$$

Graphs of several $B_k(t)$ and $P_k(t)$ are shown in FIGURES 1 and 2.

THEOREM 1. (BASIC EULER–MACLAURIN FORMULA OF ORDER p) *For any integers $n, p \geq 1$ and any function $f \in C^p[a, b]$,*

$$\sum_{i=0}^{n-1} f(a+ih)h - \int_a^b f(x) dx = \sum_{j=1}^p h^j \frac{B_j}{j!} [f^{(j-1)}(x)]_a^b + r_p(a, b, n), \tag{16a}$$

where B_j are Bernoulli coefficients, $h = (b - a)/n$, and $r_p(a, b, n)$ is the remainder of order p given by the formula

$$r_p(a, b, n) = -\frac{h^p}{p!} \int_a^b P_p\left(\frac{a-x}{h}\right) f^{(p)}(x) dx, \tag{16b}$$

where P_p is the p -th Bernoulli periodic function.

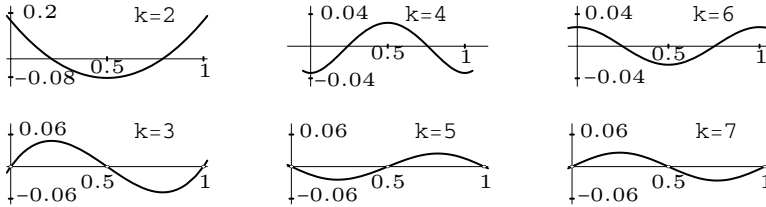


Figure 1 Bernoulli polynomials

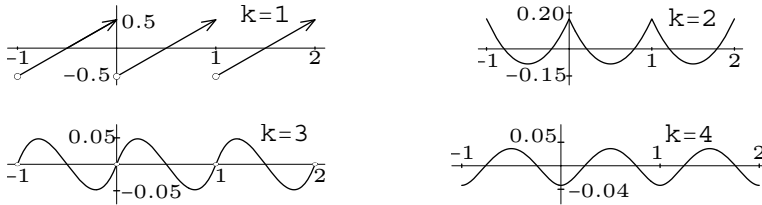


Figure 2 Bernoulli periodic functions

We arrive at the main result by replacing in (10) the functions v_k by B_k and w_k by P_k .

Formula (16a) gives the difference between a Riemann sum and the integral of a function f in terms of its derivatives at the end points of the interval of integration. (We note that it can be shown quite easily that in (16a), all the B_j with odd $j \geq 3$ actually vanish. However, for more general E–M formulas the situation is quite different; see the remarks at the end of this article.) Formulas (16b) and (13) imply a rough estimate for the remainder. If $\mu_p := \max_{0 \leq x \leq 1} |B_p(x)|$, then

$$|r_p(a, b, n)| \leq \mu_p \frac{h^p}{p!} \int_a^b |f^{(p)}(x)| dx. \tag{17}$$

For elementary applications of the E–M formula, we need some of the numbers μ_p . Equations (14) imply some basic estimates:

$$\begin{aligned} \mu_1 &= \frac{1}{2}; & \mu_2 &= \frac{1}{6}; & \mu_4 &= \mu_8 = \frac{1}{30}; & \mu_6 &= \frac{1}{42}; \\ \mu_3 &< \frac{1}{20}; & \mu_5 &< \frac{1}{35}; & \mu_7 &< \frac{1}{30}. \end{aligned} \tag{18}$$

Using μ_6 , for instance, we get

$$|r_6(a, b, n)| \leq \frac{h^6}{30240} \int_a^b |f^{(6)}(x)| dx \leq \frac{M(b-a)^7}{30240 n^6}, \tag{19}$$

where $M = \max_{a \leq x \leq b} |f^{(6)}(x)|$.

Applications of the Euler–Maclaurin formula

Numerical integration Formulas (16a) and (16b) constitute a simple and useful method of numerical integration, especially if f has easily computable derivatives through the p th order. From (16a) and (15) we read

$$\int_a^b f(x) dx = \frac{h}{2} [f(a) + f(b)] + h \sum_{i=1}^{n-1} f(a + ih) - \sum_{j=2}^p h^j \frac{B_j}{j!} [f^{(j-1)}(x)]_a^b - r_p(a, b, n).$$

This formula, together with (17) and (18), represents a good tool for numerical integration. It becomes considerably simpler in the case that $f^{(k)}(a) = f^{(k)}(b)$ for k even and less than p . (Note that $B_j = 0$ for odd $j \geq 3$.) This happens, for instance, when f is periodic with period $b - a$ ([5, p. 137]).

Let us take $p = 4$ in the preceding formula. Then (15) and (16b) give

$$\int_a^b f(x) dx = \frac{h}{2} [f(a) + f(b)] + h \sum_{i=1}^{n-1} f(a + ih) - \frac{h^2}{12} [f'(b) - f'(a)] - h^4 \frac{B_4}{4!} [f^{(3)}(x)]_a^b + \frac{h^4}{4!} \int_a^b P_4 \left(\frac{a-x}{h} \right) f^{(4)}(x) dx.$$

Substituting $x = a + th$ and writing $b = a + nh$, we can combine the last two summands:

$$\begin{aligned} & -h^4 \frac{B_4}{4!} [f^{(3)}(x)]_a^b + \frac{h^4}{4!} \int_a^b P_4 \left(\frac{a-x}{h} \right) f^{(4)}(x) dx \\ &= \frac{h^4}{4!} \int_a^b \left[P_4 \left(\frac{a-x}{h} \right) - B_4 \right] f^{(4)}(x) dx \\ &= \frac{h^5}{4!} \int_0^n [P_4(-t) - B_4] f^{(4)}(a + th) dt \\ &= \frac{h^5}{4!} f^{(4)}(\xi) \int_0^n [P_4(-t) - B_4] dt \\ &= \frac{h^5}{4!} f^{(4)}(\xi) \cdot (-nB_4) \\ &= -\frac{B_4 (b-a)^5}{4! n^4} f^{(4)}(\xi) \end{aligned}$$

at some $\xi \in [a, b]$. The third equality uses the mean value theorem. Namely, by (14), $B_4(x) - B_4 = (x - x^2)^2 \geq 0$, so, by (13) the difference $P_4(x) - B_4$ is nonnegative as well. The fourth equation follows from the fact that $\int_0^n P_4(-t) dt = 0$, according to (13) and (12). So we get *Hermite's integration formula*:

$$\int_a^b f(x) dx = s(a, b, n) + r(a, b, n), \quad (20a)$$

where

$$s(a, b, n) = \frac{h}{2} [f(a) + f(b)] + h \sum_{i=1}^{n-1} f(a + ih) - \frac{h^2}{12} [f'(b) - f'(a)] \quad (20b)$$

and, by (15),

$$r(a, b, n) = \frac{(b-a)^5}{720} f^{(4)}(\xi) \cdot n^{-4} \quad (20c)$$

for some $\xi \in [a, b]$. This remainder is about one-fourth that for Simpson's rule; the advantage is even greater if $f'(b) = f'(a)$.

Example 2. To compute $I = \int_0^2 e^{-x^2} dx$ approximately, we put $a = 0$, $b = 2$, $f(x) := e^{-x^2}$, to get $f'(x) \equiv -2xe^{-x^2}$ and $f^{(4)}(x) \equiv 4e^{-x^2}(4x^4 - 12x^2 + 3)$, and evaluate

$$M = \max \{|f^{(4)}(x)| : 0 \leq x \leq 2\} = \max \{|4e^{-t}(4t^2 - 12t + 3)| : 0 \leq t \leq 4\} = 12.$$

So by (20c) we estimate

$$|r(0, 2, n)| \leq \frac{2^5}{720} 12 \cdot n^{-4} = \frac{8}{15} n^{-4};$$

for example, $|r(0, 2, 20)| \leq 4 \times 10^{-6}$. We calculate $s(0, 2, 20) = 0.882081 + \delta$, where $0 < \delta < 10^{-6}$, and by (20a) find

$$I = 0.882081 + \delta + r(0, 2, 20) = 0.882081 + \Delta,$$

where $-4 \times 10^{-6} < \Delta \leq 5 \times 10^{-6}$. Thus $I = 0.8820 \dots$, correct to four places.

Numerical summation The E-M formula is also a notable tool for numerical summation. Let m and n be integers satisfying $1 \leq m \leq n$. Setting $a = m$, $b = n$, and $h = 1$ in (16a), we arrive at the basic E-M summation formula for a function $f \in C^p[1, \infty)$:

$$\sum_{k=m}^{n-1} f(k) = \int_m^n f(x) dx + \sum_{j=1}^p \frac{B_j}{j!} [f^{(j-1)}(x)]_m^n + \rho_p(m, n). \quad (21a)$$

By (16b) and (13) the remainder is given by

$$\rho_p(m, n) := r_p(m, n, n-m) = -\frac{1}{p!} \int_m^n P_p(-x) f^{(p)}(x) dx, \quad (21b)$$

and is estimated by

$$|\rho_p(m, n)| \leq \frac{\mu_p}{p!} \int_m^n |f^{(p)}(x)| dx, \quad (21c)$$

where $\mu_p = \max_{0 \leq x \leq 1} |B_p(x)|$. Denoting

$$S(k) := \sum_{i=1}^k f(i) \quad \text{and} \quad \sigma_p(k) := \sum_{j=1}^p \frac{B_j}{j!} f^{(j-1)}(k) \quad (22)$$

for integers k , $p \geq 1$, we can write (21a), with $n \geq m \geq 1$, as

$$S(n) = S(m - 1) + f(n) + [\sigma_p(n) - \sigma_p(m)] + \int_m^n f(x) dx + \rho_p(m, n), \quad (23)$$

where $S(0) = 0$ by definition.

This equality is the basic summation tool derived from the E–M formula. We can use (23) to compute partial sums $S(n)$ if the integral $\int_m^n f(x) dx$ is easily computable and if we can adequately estimate the integral $\int_m^n |f^{(p)}(x)| dx$ in (21c) for positive integers m and n .

Let us work out the summation formula with $p = 3$. From (15) and (22), $\sigma_3(k) = -f(k)/2 + f'(k)/12$. Now (23) implies

$$S(n) = S(m - 1) + \frac{f(m) + f(n)}{2} + \frac{f'(n) - f'(m)}{12} + \int_m^n f(x) dx + \rho_3(m, n), \quad (23a)$$

where, by (18) and (21c),

$$|\rho_3(m, n)| \leq \frac{1}{120} \int_m^n |f'''(x)| dx \quad (23b)$$

for $m \leq n$. (This explains the first formula used in the introduction.)

Euler’s constant for a function For a $C^p[1, \infty)$ function f and any positive integer n , we consider the difference $\gamma_n := \sum_{k=1}^n f(k) - \int_1^n f(x) dx$. By (23),

$$\gamma_n = f(n) + [\sigma_p(n) - \sigma_p(1)] + \rho_p(1, n), \quad n \geq 1. \quad (24a)$$

Let us assume from now on that finite limits $\lambda_0 := \lim_{n \rightarrow \infty} f(n)$ and $\lambda_k := \lim_{n \rightarrow \infty} f^{(k)}(n)$ exist for every positive integer $k \leq p - 1$ (the convergence is considered only in the sense of sequences). Let us also suppose that $\int_1^\infty |f^{(p)}(x)| dx < \infty$. By (21b) and (21c), this ensures the existence of the finite limit

$$\rho_p(m, \infty) := \lim_{n \rightarrow \infty} \rho_p(m, n) = -\frac{1}{p!} \int_m^\infty P_p(-x) f^{(p)}(x) dx \quad (24b)$$

for every integer $m \geq 1$. Our assumptions imply, according to (24a), that the limit $\gamma := \lim_{n \rightarrow \infty} \gamma_n$ (called *Euler’s constant for the function f*) exists and satisfies the equality

$$\gamma = \lambda_0 + [\sigma_p(\infty) - \sigma_p(1)] + \rho_p(1, \infty), \quad (24c)$$

where

$$\sigma_p(\infty) := \sum_{j=1}^p \frac{B_j \lambda_{j-1}}{j!}.$$

(As $B_j = 0$ for odd $j \geq 3$, we could suppose above that limit λ_k exists only for $k = 0$ and all odd $k \leq p - 1$.) Comparing (24a) and (24c), we obtain, for any integer $n \geq 1$,

$$\gamma = \gamma_n + [\lambda_0 - f(n)] + [\sigma_p(\infty) - \sigma_p(n)] + \delta_p(n), \quad (25a)$$

where $\delta_p(n) = -\frac{1}{p!} \int_n^\infty P_p(-x) f^{(p)}(x) dx$. Now (13) implies that

$$|\delta_p(n)| \leq \frac{\mu_p}{p!} \int_n^\infty |f^{(p)}(x)| dx, \quad (25b)$$

when $\mu_p = \max_{0 \leq x \leq 1} |B_p(x)|$.

Now (25a) and (25b) enable us to compute the Euler's constant γ for a function f ; knowing its numerical value, we can compute partial sums $S(n)$. Namely, since $\gamma_n := S(n) - \int_1^n f(x) dx$, formula (25a) implies that, for $n \geq 1$,

$$S(n) = \gamma + \int_1^n f(x) dx + [f(n) - \lambda_0] + [\sigma_p(n) - \sigma_p(\infty)] - \delta_p(n). \quad (26)$$

Example 3. To compute the *Euler–Mascheroni constant* γ^* , and to estimate the harmonic sum $H_n := \sum_{k=1}^n 1/k$ we use in (25a) the sum $\sigma_3(n) = -1/2n - 1/12n^2$ and limits $\lambda_k = 0$ for $k \geq 0$; thus $\sigma_3(\infty) = 0$. Now from (25a) we obtain, for $n \geq 1$,

$$\gamma^* = (H_n - \ln n) - \frac{1}{2n} + \frac{1}{12n^2} + \delta_3(n). \quad (27a)$$

Using (25b) and (18) we estimate

$$|\delta_3(n)| \leq \frac{\mu_3}{3!} \int_n^\infty |f'''(x)| dx < -\frac{1/20}{6} [f''(x)]_n^\infty = \frac{1}{120} \cdot 2n^{-3} = \frac{1}{60n^3}. \quad (27b)$$

(A more sophisticated approach results in the better estimate $-1/64n^4 \leq \delta_3(n) \leq 0$.) For example, $|\delta_3(100)| < 1.7 \times 10^{-8}$. Calculating $H_n - \ln n - 1/(2n) + 1/(12n^2)$ at $n = 100$ directly to nine places gives 0.577215664... Therefore

$$0.577215647 < \gamma^* < 0.577215682; \quad (27c)$$

that is, $\gamma^* = 0.5772156\dots$, correct to seven places. To get more correct places we need only enlarge the parameter n or p in (25a). From (27a) and (27b) we obtain the asymptotic estimates

$$\gamma^* + \ln n + \frac{1}{2n} - \frac{1}{12n^2} - \frac{1}{60n^3} < H_n < \gamma^* + \ln n + \frac{1}{2n} - \frac{1}{12n^2} + \frac{1}{60n^3}, \quad (28)$$

for $n \geq 1$, which enable us to compute harmonic sums with high precision. For example, $H_{1000^{1000}} = \gamma^* + 3000 \ln 10 + \delta$, where $|\delta| < 10^{-3000}$. According to (28) and (27c) this means $H_{1000^{1000}} = 6908.3324946\dots$, correct to seven places.

We remark that $\ln n = \sum_{k=2}^n \ln \frac{k}{k-1}$ by the telescoping method, so

$$\gamma^* = \lim_{n \rightarrow \infty} \left(\sum_{k=1}^n \frac{1}{k} + \sum_{k=2}^n \ln \frac{k}{k-1} \right) = 1 + \sum_{k=2}^{\infty} g(k),$$

where $g(x) = \frac{1}{x} + \ln \frac{x}{x-1}$. So we could also compute γ^* using the theorem below on summation of convergent series. Because the k -th derivative $g^{(k)}(x)$ decreases to 0 faster than $f^{(k)}(x)$ as $x \rightarrow \infty$, this method proves better than the previous one.

Formulas (25a) and (25b) are also of theoretical interest. They imply a theorem comparing the convergence of a series $\sum_{k=1}^{\infty} f(k)$ and an integral $\int_1^{\infty} f(x) dx$. (This theorem, known as *the integral test*, is considered in many analysis textbooks only for *monotone* functions f .) More precisely, the definition of γ_n and formula (26) implies the following result:

THEOREM 2. *If $f \in C^p[1, \infty)$, $\int_1^{\infty} |f^{(p)}(x)| dx$ converges, and finite limits $\lambda_0 := \lim_{n \rightarrow \infty} f(n)$ and $\lambda_k := \lim_{n \rightarrow \infty} f^{(k)}(n)$ exist for all positive integers $k \leq p - 1$, then*

(i) *The series $\sum_{k=1}^{\infty} f(k)$ converges if and only if the sequence $n \mapsto \int_1^n f(x) dx$ converges.*

(ii) If the series $\sum_{k=1}^{\infty} f(k)$ converges, then $\lambda_0 = 0$ and

$$\begin{aligned} \sum_{k=1}^{\infty} f(k) &= \gamma + \lim_{n \rightarrow \infty} \int_1^n f(x) dx \\ &= S(m-1) + \int_m^{\infty} f(x) dx + [\sigma_p(\infty) - \sigma_p(m)] + \delta_p(m), \end{aligned}$$

where $|\delta_p(m)| \leq \frac{\mu_p}{p!} \int_m^{\infty} |f^{(p)}(x)| dx$ for $m \geq 1$.

Example 4. From Theorem 2 we deduce easily that the series $\sum_{k=1}^{\infty} (\sin \sqrt{k})/k$ and $\sum_{k=1}^{\infty} (\sin \sqrt{k})/\sqrt{k}$ converge, setting $p = 1$ for the first series and $p = 2$ for the second. (Here we apply the comparison test for absolute convergence of improper integrals. Note that the numerical computation of sums of these two series requires a larger p , say $p = 6$ or $p = 8$. We leave details to the reader.)

Example 5. To compute $\zeta(3) = \sum_{k=1}^{\infty} 1/k^3$ we put $p = 2$ and $f(x) := x^{-3}$. From (22) and (15) we find $\sigma_2(n) = -1/2n^3 - 1/4n^4$ and $\sigma_2(\infty) = 0$. Now part (ii) of Theorem 2 gives

$$\zeta(3) = \sum_{k=1}^{m-1} \frac{1}{k^3} + \int_m^{\infty} \frac{dx}{x^3} + \frac{1}{2m^3} + \frac{1}{4m^4} + \delta_2(m),$$

where, for $m \geq 1$,

$$|\delta_2(m)| \leq \frac{\mu_2}{2} \int_m^{\infty} \frac{12}{x^5} dx = \frac{1}{4m^4}.$$

This means

$$\zeta(3) = \sum_{k=1}^{m-1} \frac{1}{k^3} + \frac{1}{2m^2} + \frac{1}{2m^3} + \Delta(m),$$

where $0 \leq \Delta(m) \leq 1/(2m^4)$ for $m \geq 2$. Since, for example, $0 \leq \Delta(20) < 4 \times 10^{-6}$, we compute

$$\sum_{k=1}^{19} \frac{1}{k^3} + \frac{1}{2 \times 20^2} + \frac{1}{2 \times 20^3} = 1.202055 \dots$$

to obtain $\zeta(3) = 1.20205 \dots$, correct to five places. For higher precision we need only use higher values of m or p in (ii) of Theorem 2. (We could also compute $\zeta(3)$ by means of Euler's constant for the function $f(x) = 1/x^3$, applying (ii) of Theorem 2.)

Remark 1 The more general E–M formula

$$\begin{aligned} h \sum_{i=0}^{n-1} f(a + (i + \omega)h) - \int_a^b f(x) dx &= \sum_{j=1}^p h^j \frac{B_j(\omega)}{j!} [f^{(j-1)}(x)]_a^b \\ &\quad - \frac{h^p}{p!} \int_a^b P_p \left(\omega - \frac{x-a}{h} \right) f^{(p)}(x) dx, \end{aligned}$$

for every $\omega \in [0, 1]$, can be deduced from (1) in the same way as was done for the equality (16a). This E–M formula expresses the difference between the integral and the Riemann integral sum for a uniform partition of $[a, b]$ and the evaluation points $a + (i + \omega)h$, $i = 0, 1, \dots, n - 1$ (see, e.g., [6, pp. 51–54]).

Remark 2 The Bernoulli coefficients B_k can be found by formal manipulation of the formula $B_k = (1 + B)^k$ for $k \geq 2$. The right side is meant to be expanded by the binomial theorem and then each power B^j is replaced by B_j . The Bernoulli polynomials can be described by applying the same process to the expression $B_k(x) = (x + B)^k$ for $k \geq 1$. Thus, this second formula is to be read

$$B_k(x) = \sum_{j=0}^k \binom{k}{j} B_{k-j} x^j,$$

where the recursion

$$B_k = -\frac{1}{k+1} \sum_{j=0}^{k-1} \binom{k+1}{j} B_j$$

for $k \geq 1$ follows formally from $B_{k+1} = (1 + B)^{k+1}$. (See [2, p. 266], [16, p. 87].)

Remark 3 By means of Fourier analysis we obtain the expansion

$$\frac{P_p(x)}{p!} = -2 \sum_{k=1}^{\infty} \frac{\cos(2k\pi x - p\frac{\pi}{2})}{(2k\pi)^p},$$

valid for all real x and every integer $p \geq 2$ [5, p. 135]. (At $p = 1$ this equality holds for every noninteger x .) From this equality we read an estimate for the so-called *Bernoulli numbers* $b_j := (-1)^{j+1} B_{2j}$:

$$2 \frac{(2j)!}{(2\pi)^{2j}} < b_j < 4 \frac{(2j)!}{(2\pi)^{2j}},$$

which holds for all $j \geq 1$. (Unfortunately, the name ‘‘Bernoulli numbers’’ is not standard in the literature.) This estimate has three consequences:

- Bernoulli coefficients alternate in sign, and are not bounded for even indices (as (15) may have suggested). (See [8, p. 452].)
- We find $\mu_p = \max \{|B_p(x)| : 0 \leq x \leq 1\} < 4 (p!) (2\pi)^{-p}$; by (17), we estimate the remainder in the E–M formula as follows:

$$|r_p(a, b, n)| \leq 4 \left(\frac{h}{2\pi}\right)^p \int_a^b |f^{(p)}(x)| dx, \quad p \geq 1.$$

- The Bernoulli numbers increase very rapidly, so it is not possible, in general, to set $p = \infty$ in the E–M formula. In fact, the series

$$\sum_{j=1}^{\infty} \frac{B_j}{j!} [f^{(j-1)}(b) - f^{(j-1)}(a)]$$

turns out to diverge for almost all functions $f(x)$ that occur in applications, regardless of a and b [11, p. 525].

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Nobody alive has done more than Gardner to spread the understanding and appreciation of mathematics, and to dispel superstition. Nobody has worked harder or more steadily to defend and enlarge this little firelit clearing we hold in the dark chittering forest of unreason.

—from John Derbyshire's review of Martin Gardner's *Did Adam and Eve Have Navels?* in *The New Criterion*.