

THE EULER-MACLAURIN SUMMATION FORMULA

We derive an expression for the *difference* between a divergent series and an infinite integral:

$$\Delta_0^\infty(f) := \left(\sum_{n=0}^{\infty} f(n) \right) - \int_0^{\infty} f(x) dx.$$

We proceed as Euler [4 , p326 et sui]:

Let $N \in \mathbb{Z}^+$. Then

$$\begin{aligned} \Delta_0^N(f) &:= \left(\sum_{n=0}^N f(n) \right) - \int_0^N f(x) dx = \\ &= 1/2[f(N) + f(0)] + \sum_{n=0}^{N-1} 1/2[f(n+1) + f(n)] - \sum_{n=0}^{N-1} \int_n^{n+1} f(x) dx = \\ &= 1/2[f(N) + f(0)] + \sum_{n=0}^{N-1} \{ 1/2[f(n+1) + f(n)] - \int_n^{n+1} f(x) dx \}. \end{aligned}$$

Now the $\{\dots\}$ term above can be re-written by an integration by parts (IBP), so that

$$\begin{aligned} \{\dots\} &= 1/2[f(n+1) + f(n)] - [xf(x)]_n^{n+1} + \int_n^{n+1} xf'(x) dx = \\ &= -(n+1/2)[f(n+1) - f(n)] + \int_n^{n+1} xf'(x) dx = \\ &= -(n+1/2) \int_n^{n+1} f'(x) dx + \int_n^{n+1} xf'(x) dx = \\ &= \int_n^{n+1} (x - n - 1/2) f'(x) dx. \end{aligned}$$

Hence

$$\Delta_0^N(f) = 1/2[f(N) + f(0)] + \sum_{n=0}^{N-1} \int_n^{n+1} (x - [x] - 1/2) f'(x) dx \quad (1)$$

where $[x]$ is the greatest integer less than x , so that

$$[x] = n \quad \forall x \in (n, n+1).$$

Now $S_1(x) := x - [x] - 1/2$ is a *sawtooth* function [5, p280] , and we define the sequence of functions

$$S_0(x), S_1(x), S_2(x), \dots$$

as follows: we let $S_0(x) := 1$, we let

$$S_k(x) = \int S_{k-1}(x) dx \quad k \in \mathbb{Z}^+ \quad , \quad (2)$$

and we choose the arbitrary constant of integration in (2) to be such that

$$\int_0^1 S_k(x) dx = 0 \quad \forall k \geq 1.$$

We defined the functions S_k as above in order to be able to integrate (1) K times by parts, where $K \in \mathbb{Z}^+$, (which assumes f to be K times differentiable), and we chose the constants of integration above so that (S_k) is a DECREASING sequence of functions, in order for our final expression for Δ_0^N - and therefore for Δ_0^∞ - to be summable.

We now proceed to integrate (1) once, twice, and by induction go to the integration K times, arriving at a preliminary expression for $\Delta_0^N(f)$ in terms of the functions S_k . The integral in (1) is expanded thus [5]:

$$\int_n^{n+1} S_1(x) f'(x) dx = [S_2(x) f'(x)]_n^{n+1} - \int_n^{n+1} S_2(x) f''(x) dx$$

where, as in (2),

$$S_2(x) = \int S_1(x) dx.$$

S_2 is the integral of 1-periodic S_1 (which has a jump discontinuity at each integer) , and

$$\int S_1(x) dx = \int x - [x] - 1/2 dx = x^2/2 - x/2 + c$$

on the interval $[0, 1)$ and hence is as above on *each* period of length 1. Hence the behaviour on each period is identical to that on the interval $[0, 1]$. So $S_2(0) = S_2(1) = c$ and

$$S_2(n+1) = S_2(n) = S_2(0) = c \quad \forall n \in \mathbb{Z}^+, \quad (3)$$

ie $S_2(x)$ is *continuous and 1-periodic*. See graphs below (Figure 1, not to scale).

Further integration by parts then gives

$$\int_n^{n+1} S_1(x) f'(x) dx = S_2(0)(f'(n+1) - f'(n)) - [S_3(x) f''(x)]_n^{n+1} + \int_n^{n+1} S_3 f'''(x) dx,$$

due to (3), and where

$$S_3(x) = \int S_2(x) dx,$$

so

$$\int_n^{n+1} S_1(x) f'(x) dx = S_2(0)(f'(n+1) - f'(n)) - S_3(0)(f''(n+1) - f''(n)) + \int_n^{n+1} S_3(x) f^{(3)}(x) dx,$$

since

$$S_3(n+1) = S_3(n) = S_3(0) \quad \forall n \in \mathbb{Z}^+, \quad (4)$$

by a similar argument as for S_2 .

FIGURE 1: $S_0(x)$, $S_1(x)$, $S_2(x)$ and $S_3(x)$ of the function sequence $S_k(x)$, $k \in \mathbb{Z}^+$. (Not to scale)

Continuing in this way, we obtain, by induction, the following expression for the K-fold integration by parts of (1):

$$\triangle_0^N(f) = 1/2[f(N) + f(0)] + \sum_{n=0}^{N-1} \left(\sum_{k=2}^{K-1} (-1)^k S_k(x) f^{(k)}(x) \Big|_n^{n+1} + (-1)^{K+1} \int_n^{n+1} S_K(x) f^{(K)}(x) dx \right),$$

ie

$$\triangle_0^N(f) = 1/2[f(N) + f(0)] + \sum_{k=2}^{K-1} (-1)^k S_k(x) f^{(k)}(x) \Big|_0^N + (-1)^{K+1} \int_0^N S_K(x) f^{(K)}(x) dx. \quad (5)$$

(see [4] , p327).

This is our preliminary expression in terms of the functions S_k , as advertised above. We must now ask what explicit form the functions S_k should or could take.

Suppose ([5], p281)

$$\sum_{k=0}^{\infty} S_k(x) t^k = G(x, t) \quad (0 \leq x < 1) \quad (6)$$

Then, since $S'_k(x) = S_{k-1}$ (from (2)), we have

$$\frac{\partial G(x, t)}{\partial x} = tG(x, t),$$

since

$$\frac{\partial G(x, t)}{\partial x} = \sum_{k=0}^{\infty} S'_k(x) t^k = \sum_{k=0}^{\infty} S_{k-1}(x) t^{k-1} t = tG(x, t).$$

This suggests $G(x, t)$ to be of the form $g(t)e^{xt}$, since

$$\frac{\partial (g(t)e^{xt})}{\partial x} = tg(t)e^{xt}.$$

Recalling condition (2) (page 2), we have

$$\begin{aligned} \int_0^1 S_k(x) dx = 0 \quad (k \geq 1) &\Rightarrow \int_0^1 G(x, t) dx = \sum_{k=0}^{\infty} \left(t^k \int_0^1 S_k(x) dx \right) = \\ &t^0 \int_0^1 S_0(x) dx = \int_0^1 1 dx = 1. \end{aligned}$$

So

$$\begin{aligned} \int_0^1 g(t)e^{xt} dx = 1 &\Rightarrow \frac{g(t)e^{xt}}{t} \Big|_0^1 = 1 \\ &\Rightarrow g(t) = \frac{t}{e^t - 1}. \end{aligned}$$

Hence

$$\sum_{k=0}^{\infty} S_k(x) t^k = \frac{te^{xt}}{e^t - 1}.$$

Now, the *BERNOULLI POLYNOMIALS* are defined by the following expansion

$$\frac{te^{xt}}{e^t - 1} =: \sum_{k=0}^{\infty} B_k(x) \frac{t^k}{k!} \quad \forall x \in \mathfrak{R}, |t| < 2\pi. \quad (7)$$

Hence

$$S_k(x) = \frac{B_k(x - [x])}{k!}.$$

We have $B_k(x - [x])$ on the rhs since our expansion (7) is then defined for the interval $[0, 1)$ as our construction implies the S_k are polynomials of degree k in the interval $[0, 1)$ ([5], p281).

So let ([4], p327)

$$S_k(x) = \frac{B_k(x)}{k!}, \quad k \in \mathbb{Z}^+ \quad (8)$$

on $(0, 1)$ and 1-periodic thereafter.

We have now defined our functions S_k explicitly, in terms of the standard Bernoulli polynomials, whose useful and relevant properties we now explore.

First, we prove the following

PROPOSITION 1

$$\frac{B'_k(x)}{k!} = \frac{B_{k-1}(x)}{(k-1)!} \quad \forall \quad k \geq 1.$$

Proof

We have

$$\frac{te^{xt}}{e^t - 1} =: \sum_{k=0}^{\infty} \frac{B_k(x)t^k}{k!}$$

Differentiating wrt x gives

$$t \frac{te^{xt}}{e^t - 1} = \sum_{k=0}^{\infty} \frac{B'_k(x)t^k}{k!},$$

so

$$t \sum_{k=0}^{\infty} \frac{B_k(x)t^k}{k!} = \sum_{k=0}^{\infty} \frac{B'_k(x)t^k}{k!},$$

so

$$\sum_{k=0}^{\infty} \frac{B_k(x)t^k}{k!} = \sum_{k=0}^{\infty} \frac{B'_k(x)t^{k-1}}{k!}.$$

But

$$\sum_{k=1}^{\infty} \frac{B_{k-1}(x)t^{k-1}}{(k-1)!} = \sum_{k=0}^{\infty} \frac{B_k(x)t^k}{k!} = \sum_{k=0}^{\infty} \frac{B'_k(x)t^{k-1}}{k!}.$$

Hence equating coefficients of t in the above expression gives us

$$\frac{B'_k(x)}{k!} = \frac{B_{k-1}(x)}{(k-1)!} \quad \forall \quad k \geq 1 \quad QED.$$

Next we introduce the *BERNOULLI NUMBERS* $B_k := B_k(0)$. We prove that

PROPOSITION 2

$$B_k(x) = \sum_{j=0}^k \binom{k}{j} B_{k-j} x^j. \quad \forall \quad k \geq 0.$$

Proof

We have

$$\frac{te^{0t}}{e^t - 1} = \sum_{k=0}^{\infty} \frac{B_k(0)t^k}{k!} \Rightarrow \frac{t}{e^t - 1} = \sum_{k=0}^{\infty} \frac{B_k t^k}{k!},$$

so

$$e^{xt} \sum_{k=0}^{\infty} \frac{B_k t^k}{k!} = \frac{te^{xt}}{e^t - 1} = \sum_{k=0}^{\infty} \frac{B_k(x)t^k}{k!}.$$

Equating coefficients of powers of t in the above expression, we have ([5],p282)

$$e^{xt} B_0 = B_0(x),$$

$$e^{xt} B_1 t = B_1(x)t,$$

and for positive integer k we have

$$e^{xt} B_k t = B_k(x)t.$$

So $B_k = B_k(0)$, as above!

Now, using Proposition 1, $B'_k(x) = kB_{k-1}(x)$, and by (8), we have

$$B_0(x) = 1,$$

so

$$B_0 = B_0(0) = 1$$

so

$$B_1(x) = \int_0^1 1 B_0 dx = B_0 x|_0^1 = B_0$$

and

$$B_1(x) = \int B_0 dx = B_0 x + c$$

so

$$B_1(0) = B_1 = c$$

so

$$B_1(x) = B_0 x + B_1$$

ie

$$B_1(x) = \binom{1}{0} B_{1-0} x^0 + \binom{1}{1} B_{1-1} x^1 = \sum_{j=0}^1 \binom{1}{j} B_{1-j} x^j.$$

Similarly,

$$B_2(x) = B_0 x^2 + 2B_1 x + B_2 = \binom{2}{0} B_{2-0} x^0 + \binom{2}{1} B_{2-1} x^1 + \binom{2}{2} B_{2-2} x^2 = \sum_{j=0}^2 \binom{2}{j} B_{2-j} x^j.$$

So, by induction, we have the required result:

$$B_k(x) = \sum_{j=0}^k \binom{k}{j} B_{k-j} x^j. \quad QED. \quad (9)$$

So far so good, but (9) is only useful if we know what the Bernoulli numbers are! We now derive an algorithm for recursively extracting the Bernoulli numbers:

Now, ([5],282), (7) is unchanged if we simultaneously replace x and t by $1-x$ and $-t$ respectively, hence

$$B_k(1-x) = (-1)^k B_k(x). \quad (10)$$

Moreover, apart from B_1 , all the Bernoulli numbers with an odd suffix are equal to zero. This is because

$$\frac{t}{e^t - 1} + t/2 = \left(\sum_{k=0}^{\infty} B_k \frac{t^k}{k!} \right) + t/2$$

is an *even* function of t , so odd powers of $-t$ must vanish from the series on the rhs of the above expression, (as the function on lhs above is ≥ 0 for positive t) beyond a certain value of k . (10) becomes:

$$B_k(1-0) = (-1)^k B_k(0)$$

ie

$$B_k(1) = B_k \quad (k \geq 2). \quad (11)$$

So let $x = 1$ in (9) and we have

$$B_k(1) = B_k = \sum_{j=0}^k \binom{k}{j} B_{k-j} \Rightarrow B_k = \sum_{j=0}^k \binom{k}{k-j} B_{k-j} = \sum_{j=0}^k \binom{k}{j} B_j,$$

by first recalling that $\binom{k}{j} = \binom{k}{k-j}$, and secondly just re-labelling $k-j$ as j .

So

$$\begin{aligned} B_k &= \binom{k}{0} B_0 + \binom{k}{1} B_1 + \cdots + \binom{k}{k} B_k \\ \Rightarrow B_k - \binom{k}{k} B_k &= 0 = \binom{k}{0} B_0 + \cdots + \binom{k}{k-1} B_{k-1}, \\ &\Rightarrow -\binom{k}{k-1} B_{k-1} = \sum_{j=0}^{k-2} \binom{k}{j} B_j, \end{aligned}$$

which gives us the promised algorithm for recursively calculating the B_k as

$$B_{k-1} = -1/k \sum_{j=0}^{k-2} \binom{k}{j} B_j \quad (k \geq 2).$$

Hence, recalling that $B_0 = 1$, we have ([5] p282)

$$B_1 = -1/2, \quad B_2 = 1/6, \quad B_3 = 0, \quad B_4 = -1/30, \dots$$

So, by (11), we have that the Bernoulli polynomials are 1-periodic, as $B_k(0) = B_k = B_k(1)$. They are continuous as they are polynomials, and we will now see that successive Bernoulli polynomials have increasing powers of x , and so, on $[0, 1)$, this means that they also fulfil our requirement that the S_k be a DECREASING sequence of functions:

So, from Proposition 2, the first seven Bernoulli polynomials are :

$$B_0(x) = 1, \quad B_1(x) = x - 1/2, \quad B_2(x) = x^2 - x + 1/6, \quad B_3(x) = x^3 - (3/2)x^2 + (1/2)x,$$

$$B_4(x) = x^4 - 2x^3 + x^2 - 1/30, \quad B_5(x) = x^5 - (5/2)x^4 + (5/3)x^3 - (1/6)x,$$

$$B_6(x) = x^6 - 3x^5 + (5/2)x^4 - (1/2)x^2 + 1/42$$

Hence, from all the above discussion of Bernoulli polynomials, (5) now becomes:

$$\triangle_0^N(f) = 1/2[f(N) + f(0)] + \sum_{k=2}^{K-1} \frac{(-1)^k B_k(x) f^{(k)}(x)|_0^N}{k!} + (-1)^{K+1} \int_0^N \frac{B_K(x) f^{(K)}(x)}{K!} dx.$$

From our remarks about Bernoulli numbers of odd suffix vanishing, and remembering that the second term above is an integration between *integer* values, so (11) applies and we can take the Bernoulli term out as a Bernoulli number, we have

$$\Delta_0^N(f) = 1/2[f(N)+f(0)] + \sum_{m=1}^{M(K)} \frac{B_{2m}}{(2m)!} \left[f^{(2m-1)}(x) \right]_0^N + (-1)^{K+1} \int_0^N \frac{B_K(x) f^{(K)}(x)}{K!} dx.$$

Where

$$M(K) := K/2, \ K \text{ even, and } M(K) := (K-1)/2, \ K \text{ odd.}$$

It will be noticed that we have kept only the odd derivatives of f. This is because, in the above summation, we would lose either all even or all odd derivatives of f, since all odd Bernoulli numbers vanish above B_1 . So we choose to keep the odd derivatives. This condition will preserve the first derivative of f.