Euler-Maclaurin summation formula

Lecture notes by M. G. Rozman

Last modified: March 29, 2016

Euler-Maclaurin summation formula gives an estimation of the sum $\sum_{i=n}^{N} f(i)$ in terms of the integral $\int_n^N f(x)\mathrm{d}x$ and "correction" terms. It was discovered independently by Euler and Maclaurin and published by Euler in 1732, and by Maclaurin in 1742.

The presentation below follows[1], [2, Ch Y], [3, Ch 1].

1 Preliminaries. Bernoulli numbers

The Bernoulli numbers B_n are *rational* numbers that can be defined as coefficients in the following power series expansion:

$$\frac{x}{e^x - 1} = \sum_{n=0}^{\infty} B_n \frac{x^n}{n!}. \tag{1}$$

These numbers are important in number theory, analysis, and differential topology.

Unless you are using a computer algebra system for series expansion [1] it is not easy to find the coefficients in the right hand side of Eq. (1). However, it is easy to write Taylor series for the reciprocal of the left hand side of Eq. (1):

$$\frac{e^x - 1}{x} = \frac{1}{x}\sum_{k=1}^{\infty} \frac{x^k}{k!} = \sum_{k=0}^{\infty} \frac{x^k}{(k+1)!} = 1 + \frac{x}{2} + \frac{x^2}{6} + \frac{x^3}{24} + \ldots. \tag{2}$$

Thus, the Bernoulli numbers can be computer recurrently by equating to zero the coefficients at positive powers of x in the identity

$$\begin{aligned} 1 &= \frac{x}{e^x - 1} \cdot \frac{e^x - 1}{x} = \sum_{n,k=0}^{\infty} \frac{B_n}{(k+1)!\, n!}\, x^{k+n} \\ &= \left(1 + \frac{x}{2} + \frac{x^2}{6} + \frac{x^3}{24} + \ldots\right) \cdot \left(B_0 + \frac{B_1}{1!}x + \frac{B_2}{2!}x^2 + \ldots\right) \\ &= B_0 + \left(\frac{B_0}{2!\,0!} + \frac{B_1}{1!\,1!}\right)x + \left(\frac{B_0}{3!\,0!} + \frac{B_1}{2!\,1!} + \frac{B_2}{1!\,2!}\right)x^2 + \ldots. \end{aligned} \tag{3}$$

[1]For example, `Series[x/(Exp[x] - 1), x, 0, 6]` in Mathematica

From here, $B_0 = 1$, $B_1 = -\frac{1}{2}B_0 = -\frac{1}{2}$, $B_2 = -\frac{1}{3}B_0 - B_1 = \frac{1}{6}$, etc.

$$B_1 = -\frac{1}{2} \tag{4}$$

is the only non-zero Bernoulli number with an odd subscript. The first Bernoulli numbers with even subscripts are as following:

$$B_0 = 1, \quad B_2 = \frac{1}{6}, \quad B_4 = -\frac{1}{30}, \quad B_6 = \frac{1}{42}, \quad B_8 = -\frac{1}{30}, \quad B_{10} = \frac{5}{66}, \quad \ldots . \tag{5}$$

The first few terms in the Expansion Eq. (1) are as following:

$$\frac{x}{e^x - 1} = 1 - \frac{x}{2} + \frac{x^2}{12} - \frac{x^4}{720} + \frac{x^6}{30240} - \frac{x^8}{1209600} + \frac{x^{10}}{47900160} + \ldots . \tag{6}$$

2 Preliminaries. Operators $\hat{D}$ and $\hat{T}$

If $f(x)$ is a "good" function (meaning that we can apply formulas of differential calculus without 'reservations'), then the correspondence

$$f(x) \longrightarrow f'(x) \equiv \frac{\mathrm{d}}{\mathrm{d}x} f(x) \tag{7}$$

can be regarded as the *operator of differentiation*

$$\hat{D} \equiv \frac{\mathrm{d}}{\mathrm{d}x} \tag{8}$$

that act on the function and transforms it into derivative. Given $\hat{D}$, we can naturally define the powers of the operator of differentiation

$$\hat{D}^2 f(x) = \hat{D}\left(\hat{D} f(x)\right) = \frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}x} f(x) = \frac{\mathrm{d}^2}{\mathrm{d}x^2} f(x) \quad \text{i.e.} \quad \hat{D}^2 = \frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{9}$$

or in general,

$$\hat{D}^n = \frac{\mathrm{d}^n}{\mathrm{d}x^n}. \tag{10}$$

We can define functions of the operator of differentiation as following: if $g(x)$ is a "good" function that can be expanded into power series,

$$g(x) = \sum_{n=0}^{\infty} a_n x^n, \tag{11}$$

then the operator function $g(\hat{D})$ is defined as following.

$$g(\hat{D}) = \sum_{n=0}^{\infty} a_n \hat{D}^n \tag{12}$$

Let's consider the exponential function of the differential operator:

$$\hat{T} \equiv e^{\hat{D}} = \sum_{n=0}^{\infty} \frac{\hat{D}^n}{n!}. \tag{13}$$

When applied to a "good" function $f(x)$,

$$\hat{T} f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\hat{D}^n f(x)\right) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\mathrm{d}^n f}{\mathrm{d}\, x^n}. \tag{14}$$

The last expression in Eq. (14) is just a Taylor series for $f(x+1)$. Thus,

$$\hat{T} f(x) = f(x+1). \tag{15}$$

and $\hat{T}$ can be regarded as the *shift operator*. Shifting by 2 can be considered as a composition of two shift by one operations:

$$f(x+2) = \hat{T} f(x+1) = \hat{T}\left(\hat{T} f(x)\right) = \hat{T}^2 f(x). \tag{16}$$

Similarly, shifting by a positive value s can be considered as the result of operator $\hat{T}^s$:

$$f(x+s) = \hat{T}^s f(x). \tag{17}$$

3 Summation of series in terms of operator $\hat{D}$

We can now formally write

$$\begin{aligned} \sum_{n=0}^{\infty} f(x+n) &= f(x) + f(x+1) + f(x+2) + \ldots = f(x) + \hat{T} f(x) + \hat{T}^2 f(x) + \ldots \\ &= \left(1 + \hat{T} + \hat{T}^2 + \ldots\right) f(x) = \frac{1}{1-\hat{T}} f(x) = \frac{1}{1-e^{\hat{D}}} f(x), \end{aligned} \tag{18}$$

where the expression for the sum of geometric progression was used.

Treating $\hat{D}$ as an ordinary variable, and using Bernoulli numbers, we obtain the expansion:

$$\begin{aligned} \frac{1}{1-e^{\hat{D}}} &= -\frac{1}{\hat{D}} \frac{\hat{D}}{e^{\hat{D}}-1} = -\frac{1}{\hat{D}}\left(1 - \frac{1}{2}\hat{D} + \sum_{n=2}^{\infty} \frac{B_n}{n!} \hat{D}^n\right) \\ &= -\frac{1}{\hat{D}} + \frac{1}{2} - \sum_{n=2}^{\infty} \frac{B_n}{n!} \hat{D}^{n-1} \end{aligned} \tag{19}$$

The question remaining before Eq. (19) can be applied is what does $\hat{D}^{-1}$ mean.

It is natural to assume that $\hat{D}$ satisfies the relation

$$\hat{D}\left(\frac{1}{\hat{D}} f(x)\right) = \frac{\hat{D}}{\hat{D}} f(x) = f(x). \tag{20}$$

Therefore $\frac{1}{\hat{D}}$ has to be an inverse operator to differentiation, that is integration.

$$\frac{1}{\hat{D}} f(x) = \int f(x)\,\mathrm{d}x + C. \tag{21}$$

We still need to fix an integration constant i.e. to chose the integration limits. As we see later, we obtain consistent results, if

$$\frac{1}{\hat{D}} f(x) = \int_{\infty}^{x} f(x)\,\mathrm{d}x, \tag{22}$$

or

$$-\frac{1}{\hat{D}} f(x) = \int_{x}^{\infty} f(x)\,\mathrm{d}x. \tag{23}$$

Collecting the results together,

$$\sum_{n=0}^{\infty} f(x+n) = \int_{x}^{\infty} f(x)\,\mathrm{d}x + \frac{1}{2} f(x) - \sum_{n=2}^{\infty} \frac{B_n}{n!} \frac{\mathrm{d}^{n-1} f(x)}{\mathrm{d}\ x^{n-1}}. \tag{24}$$

4 The Euler-Maclaurin summation formula

Equation (24) is the Euler-Maclaurin summation formula. It can be rewritten for the case of a finite sum as following:

$$\begin{aligned}
\sum_{k=n}^{N} f(k) &= \sum_{k=n}^{\infty} f(k) - \sum_{k=N+1}^{\infty} f(k) \\
&= \sum_{k=n}^{\infty} f(k) - \sum_{k=N}^{\infty} f(k) + f(N) \\
&= \sum_{k=0}^{\infty} f(k+n) - \sum_{k=0}^{\infty} f(k+N) + f(N) \\
&= \int_{n}^{\infty} f(x)\,\mathrm{d}x - \int_{N}^{\infty} f(x)\,\mathrm{d}x + \frac{1}{2} f(n) - \frac{1}{2} f(N) + f(N) \\
&\quad + \sum_{n=2}^{\infty} \frac{B_n}{n!} \frac{\mathrm{d}^{n-1} f(n)}{\mathrm{d}\ x^{n-1}} + \sum_{n=2}^{\infty} \frac{B_n}{n!} \frac{\mathrm{d}^{n-1} f(N)}{\mathrm{d}\ x^{n-1}} \\
&= \int_{n}^{N} f(x)\,\mathrm{d}x + \frac{1}{2}\left[f(n) + f(N)\right] + \sum_{n=2}^{\infty} \frac{B_n}{n!} \left[\left.\frac{\mathrm{d}^{n-1} f}{\mathrm{d}\,x^{n-1}}\right|_{x=N} - \left.\frac{\mathrm{d}^{n-1} f}{\mathrm{d}\,x^{n-1}}\right|_{x=n} \right].
\end{aligned} \tag{25}$$

5 Stirling's formula

As an application of Euler-Maclaurin summation formula, let's consider the Stirling's approximation for $\Gamma(n)$ for positive integer $n \gg 1$.

$$\Gamma(n+1) = n!, \tag{26}$$

$$\ln\Big(\Gamma(n+1)\Big) = \ln n! = \ln\Big(1\cdot 2\cdot 3\cdot \ldots \cdot (n-1)\cdot n\Big) = \sum_{k=1}^{n} \ln k. \tag{27}$$

The first two terms in Eq. (25) give us the following approximation:

$$\begin{aligned}
\ln\Big(\Gamma(n+1)\Big) = \ln(n!) &= \int_1^n \ln(x)\,\mathrm{d}x + \frac{1}{2}\left(\ln(1) + \ln(n)\right) \\
&= x\ln(x)|_1^n - \int_1^n \frac{x}{x}\,\mathrm{d}x + \frac{1}{2}\ln(n) \\
&= n\ln(n) - n + 1 + \frac{1}{2}\ln(n).
\end{aligned} \tag{28}$$

The next correction requires more efforts.

Let's notice first that the term with the derivatives of $\ln(x)$ at $x = n$ in Eq. (25) are proportional to negative powers of n and thus $\to 0$ as $n \to \infty$. On the other hand, the sum of the term with the derivatives of $\ln(x)$ at $x = 1$ is a constant independent of n. Thus,

$$\ln\Gamma(n+1) = \ln n! = \ln\left(\frac{n}{e}\right)^n + \ln\sqrt{n} + \ln(C) = \ln\left[C\sqrt{n}\left(\frac{n}{e}\right)^n\right], \tag{29}$$

or

$$\Gamma(n+1) = n! = C\sqrt{n}\left(\frac{n}{e}\right)^n = Cn^{n+\frac{1}{2}}e^{-n}. \tag{30}$$

In order to find the constant in Eq. (30), we are going to use the duplication formula for Gamma function, Eq. (47). We first rewrite eq. (47) as following:

$$\Gamma(2n+1) = \frac{2^{2n}}{\sqrt{\pi}}\Gamma(n+1)\,\Gamma\left(n+\frac{1}{2}\right), \tag{31}$$

or

$$(2n)! = \frac{2^{2n}}{\sqrt{\pi}}n!\,\Gamma\left(n+\frac{1}{2}\right), \tag{32}$$

Let's accept without proof that Eq. (30) that we derived for integer n works also for any large positive argument. Indeed, if Eq. (30) is a good approximation for $\Gamma(n)$ and for $\Gamma(n+1)$ it is reasonable to assume that it works in between n and $n+1$. Therefore,

$$\Gamma\left(n+\frac{1}{2}\right) = \Gamma\left(n-\frac{1}{2}+1\right) \approx C\left(n-\frac{1}{2}\right)^n e^{-n+\frac{1}{2}}. \tag{33}$$

For $n \gg 1$,

$$\left(n-\frac{1}{2}\right)^n = n^n \left\{\left(1-\frac{1}{2n}\right)^{2n}\right\}^{\frac{1}{2}} \approx n^n e^{-\frac{1}{2}}. \tag{34}$$

Thus,

$$\Gamma\left(n+\frac{1}{2}\right) \approx C n^n e^{-n}. \tag{35}$$

Substituting Eq. (30), (35) into Eq. (32), we obtain:

$$C\,(2n)^{2n+\frac{1}{2}}\,e^{-2n} = \frac{2^{2n}}{\sqrt{\pi}}\,C n^{n+\frac{1}{2}} e^{-n}\,C n^n e^{-n}. \tag{36}$$

After simplification,

$$C = \sqrt{2\pi}. \tag{37}$$

Finally,

$$\Gamma(n+1) = n! = \sqrt{2\pi n}\left(\frac{n}{e}\right)^n = \sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n}. \tag{38}$$

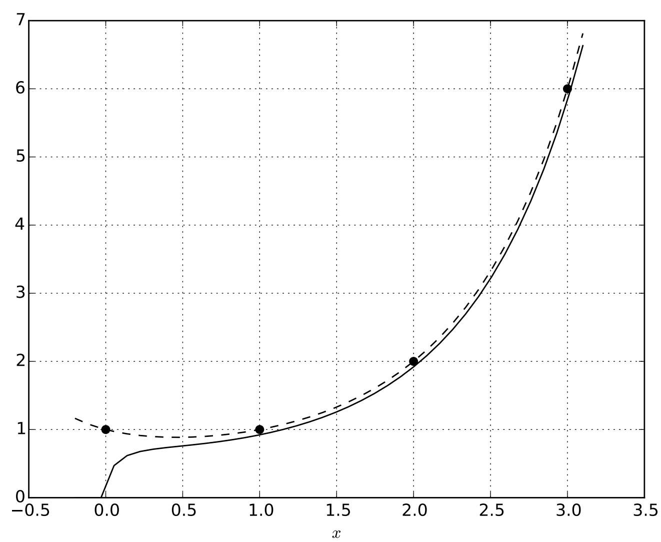

Figure 1: Stirling's approximation Eq. (38), solid line, compared with Gamma function, dashed line, and factorial, circular markers.

6 Examples

Example 1. Lets consider the following sum:

$$S(\alpha, k) = \sum_{n=-\infty}^{\infty} e^{-\alpha (n^2)^k}, \quad \alpha > 0,\ k > 0. \tag{39}$$

The case of small α, $\alpha \ll 1$, is most difficult for a numerical summation, since many terms need to be added in the sum Eq. (39). Small α is where the Euler-Maclaurin approximation works the best.

$$S(\alpha,k) \approx \int_{-\infty}^{\infty} e^{-\alpha(x^2)^k}\,\mathrm{d}x = \int_{0}^{\infty} e^{-\alpha x^{2k}}\,\mathrm{d}x. \tag{40}$$

Introduction of a new integration variable,

$$u = \alpha x^{2k} \quad \to \quad x = \left(\frac{u}{\alpha}\right)^{\frac{1}{2k}} \quad \to \quad \mathrm{d}x = \frac{1}{2k}\alpha^{-\frac{1}{2k}} u^{\frac{1}{2k}-1}\mathrm{d}u, \tag{41}$$

transforms the integral as following:

$$\frac{1}{k}\alpha^{-\frac{1}{2k}} \int_{0}^{\infty} e^{-u} u^{-\frac{1}{2k}} u^{\frac{1}{2k}-1}\,\mathrm{d}u = \frac{\alpha^{-\frac{1}{2k}}}{k}\Gamma\left(\frac{1}{2k}\right), \tag{42}$$

so that

$$S(\alpha,k) \approx \frac{\alpha^{-\frac{1}{2k}}}{k}\Gamma\left(\frac{1}{2k}\right). \tag{43}$$

The approximation Eq. (43) is compared with the results of numerical calculations in Fig. 2 and Fig. 3.

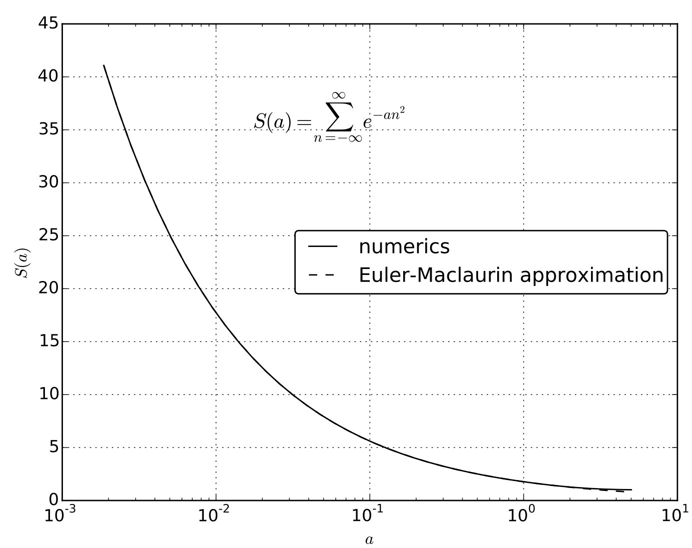

Figure 2: Euler-Maclaurin approximation Eq. (43), dashed line, compared with numerical value of the sum $S(\alpha,1)$, solid line.

Example 2. Euler-Maclaurin summation formula can produce exact expression for the sum if $f(x)$ is a polynomial. Indeed, in this case only finite number of derivatives of $f(x)$ is non zero. Thus there is only a finite number of 'correction' terms in Eq. (25).

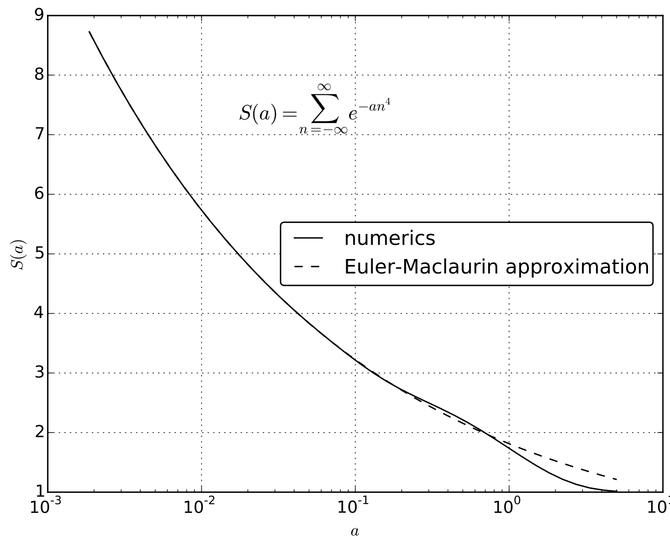

Figure 3: Euler-Maclaurin approximation Eq. (43), dashed line, compared with numerical value of the sum $S(\alpha, 2)$, solid line.

Let's consider the following sum:

$$S_3 \equiv \sum_{k=1}^{n} k^3. \tag{44}$$

Euler-Maclaurin expression for the sum is exactly as following,

$$\begin{aligned} S_3 &= \int_1^n x^3 \,\mathrm{d}x + \frac{1}{2}\left(n^3+1\right) + \frac{B_2}{2}\left(3n^2-3\right) + \frac{B_4}{4!}\left(6-6\right) \\ &= \frac{1}{4}\left(n^4-1\right) + \frac{1}{2}\left(n^3+1\right) + \frac{1}{4}\left(n^2-1\right), \end{aligned} \tag{45}$$

where we used $B_2 = \frac{1}{6}$. After some algebra,

$$S_3 = \frac{1}{4} n^2 (n+1)^2, \tag{46}$$

which is indeed the correct result.

Appendix A. Duplication formula for Gamma function

The duplication formula for the Gamma function is

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}} \Gamma(z)\, \Gamma\left(z+\frac{1}{2}\right) \tag{47}$$

It is also called the Legendre duplication formula.

We start from the definition of Beta function, $B(z,z)$.

$$B(z,z) = \int_0^1 x^{z-1}(1-x)^{z-1}\mathrm{d}x. \tag{48}$$

Let's change the integration variable to t, $x = \frac{1+t}{2}$, so that $-1 \le t \le 1$ and $\mathrm{d}x = \frac{1}{2}\mathrm{d}t$. This transforms Eq. (48) into

$$B(z,z) = 2^{2-2z}\,\frac{1}{2}\int_{-1}^{1}(1-t)^{z-1}(1+t)^{z-1}\mathrm{d}t = 2^{2-2z}\int_0^1 (1-t^2)^{z-1}\mathrm{d}t. \tag{49}$$

Changing the integration variable in the last integral to $u = t^2$, so that $0 \le u \le 1$ and $\mathrm{d}t = \frac{1}{2}u^{-\frac{1}{2}}$, we transform the integral to

$$B(z,z) = 2^{1-2z}\int_0^1 u^{-\frac{1}{2}}(1-u)^{z-1}\mathrm{d}u = 2^{1-2z}B\left(\frac{1}{2},z\right), \tag{50}$$

i.e.

$$B(z,z) = 2^{1-2z}B\left(\frac{1}{2},z\right). \tag{51}$$

In terms of Gamma function,

$$B(z,z) = \frac{\Gamma(z)\,\Gamma(z)}{\Gamma(2z)}, \tag{52}$$

$$B\left(\frac{1}{2},z\right) = \frac{\Gamma\left(\frac{1}{2}\right)\Gamma(z)}{\Gamma\left(z+\frac{1}{2}\right)}, \tag{53}$$

so that

$$\frac{\Gamma(z)\Gamma(z)}{\Gamma(2z)} = 2^{1-2z}\frac{\Gamma\left(\frac{1}{2}\right)\Gamma(z)}{\Gamma\left(z+\frac{1}{2}\right)}. \tag{54}$$

Rearranging, and using the value of $\Gamma(1/2) = \sqrt{\pi}$, we see that

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}}\Gamma(z)\Gamma\left(z+\frac{1}{2}\right), \tag{55}$$

which is the duplication formula.

References

[1] Sergey Sadov. Euler's derivation of the euler-maclaurin formula, 2003. URL http://www.math.mun.ca/~sergey/Winter03/m3132/Asst8/eumac.pdf. [Online; accessed 2016-03-24].

[2] Sanjoy Mahajan. *Street-Fighting Mathematics: The Art of Educated Guessing and Opportunistic Problem Solving*. MIT Press, 2010.

[3] Hung Cheng. *Advanced Analytic Methods in Applied Mathematics, Science, and Engineering*. LuBan Press, 2007.