EULER–MACLAURIN SUMMATION FORMULA

LECTURE NOTES, SPRING SEMESTER 2017

http://www.phys.uconn.edu/~rozman/Courses/P2400_17S/

Euler–Maclaurin summation formula gives an estimation of the sum \( \sum_{i=n}^{N} f(i) \) in terms of the integral \( \int_{n}^{N} f(x) dx \) 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. 6.3], [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

\(^{1}\)For example, Series[x/(Exp[x] - 1), x, 0, 6] in Mathematica
for the reciprocal of the left hand side of Eq. (1):

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

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

\[ 1 = \frac{e^x - 1}{x} \cdot \left(1 + \frac{x}{2} + \frac{x^2}{6} + \frac{x^3}{24} + \ldots\right) \cdot \left(B_0 + \frac{B_1}{1!} x + \frac{B_2}{2!} x^2 + \ldots\right) \]

\[ = B_0 + \left(\frac{B_0}{2!0!} + \frac{B_1}{1!1!}\right) x + \left(\frac{B_0}{3!0!} + \frac{B_1}{2!1!} + \frac{B_2}{1!2!}\right) x^2 + \ldots \] (3)

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

\[ B_1 = -\frac{1}{2} \] (4)

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

\[ B_0 = 1, \quad B_2 = \frac{1}{6}, \quad B_4 = -\frac{1}{30}, \quad B_6 = \frac{1}{42}, \quad B_8 = -\frac{1}{30}, \quad B_{10} = \frac{5}{66}, \ldots \] (5)

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

\[ \frac{x}{e^x - 1} = 1 - \frac{x}{2} + \frac{x^2}{12} - \frac{x^4}{720} + \frac{x^6}{30240} - \frac{x^8}{1209600} + \frac{x^{10}}{47900160} + \ldots \] (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

\[ f(x) \rightarrow f'(x) \equiv \frac{d}{dx} f(x) \] (7)

can be regarded as the operator of differentiation

\[ \hat{D} \equiv \frac{d}{dx} \] (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

\[
\hat{D}^2 f(x) = \hat{D} \left( \hat{D} f(x) \right) = \frac{d}{dx} \frac{d}{dx} f(x) = \frac{d^2}{dx^2} f(x)
\]

i.e. \( \hat{D}^2 = \frac{d^2}{dx^2} \), \( n = 2 \),

or in general,

\[
\hat{D}^n = \frac{d^n}{dx^n}.
\]

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,

\[
g(x) = \sum_{n=0}^{\infty} a_n x^n,
\]

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

\[
g(\hat{D}) = \sum_{n=0}^{\infty} a_n \hat{D}^n
\]

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

\[
\hat{T} \equiv e^{\hat{D}} = \sum_{n=0}^{\infty} \frac{\hat{D}^n}{n!}.
\]

When applied to a “good” function \( f(x) \),

\[
\hat{T} f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left( \hat{D}^n f(x) \right) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}
\]

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

\[
\hat{T} f(x) = f(x + 1).
\]

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:

\[
f(x + 2) = \hat{T} f(x + 1) = \hat{T} \left( \hat{T} f(x) \right) = \hat{T}^2 f(x).
\]

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

\[
f(x + s) = \hat{T}^s f(x).
\]
3 Summation of series in terms of operator $\hat{D}$

We can now formally write

$$\sum_{n=0}^{\infty} f(x + n) = f(x) + f(x + 1) + f(x + 2) + \ldots = f(x) + \hat{T} f(x) + \hat{T}^2 f(x) + \ldots$$

$$= \left(1 + \hat{T} + \hat{T}^2 + \ldots\right) f(x) = \frac{1}{1 - \hat{T}} f(x) = \frac{1}{1 - e^{\hat{D}}} f(x), \quad (18)$$

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:

$$\frac{1}{1 - e^{\hat{D}}} = -\frac{1}{\hat{D}} \frac{\hat{D}}{e^{\hat{D}} - 1} = -\frac{1}{\hat{D}} \left(1 - \frac{1}{2} \hat{D} + \sum_{n=2}^{\infty} \frac{B_n}{n!} \hat{D}^n\right)$$

$$= -\frac{1}{\hat{D}} + \frac{1}{2} - \sum_{n=2}^{\infty} \frac{B_n}{n!} \hat{D}^{n-1}. \quad (19)$$

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

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

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

$$\frac{1}{\hat{D}} f(x) = \int f(x) \, dx + C. \quad (21)$$

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

$$\frac{1}{\hat{D}} f(x) = \int_{\infty}^{x} f(x) \, dx, \quad (22)$$

or

$$-\frac{1}{\hat{D}} f(x) = \int_{x}^{\infty} f(x) \, dx. \quad (23)$$
Collecting the results together,

\[
\sum_{n=0}^{\infty} f(x + n) = \int f(x) \, dx + \frac{1}{2} f(x) - \sum_{n=2}^{\infty} \frac{B_n}{n!} \frac{d^{n-1} f(x)}{d x^{n-1}}.
\]  

(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:

\[
\sum_{k=n}^{N} f(k) = \sum_{k=n}^{\infty} f(k) - \sum_{k=N+1}^{\infty} f(k)
\]

\[
= \sum_{k=n}^{\infty} f(k) - \sum_{k=N}^{\infty} f(k) + f(N)
\]

\[
= \sum_{k=0}^{\infty} f(k + n) - \sum_{k=0}^{\infty} f(k + N) + f(N)
\]

\[
= \int_{n}^{\infty} f(x) \, dx - \int_{N}^{\infty} f(x) \, dx + \frac{1}{2} f(n) - \frac{1}{2} f(N) + f(N)
\]

\[
+ \sum_{n=2}^{\infty} \frac{B_n}{n!} \frac{d^{n-1} f(n)}{d x^{n-1}} + \sum_{n=2}^{\infty} \frac{B_n}{n!} \frac{d^{n-1} f(N)}{d x^{n-1}}
\]

\[
= \sum_{k=n}^{N} f(x) \, dx + \frac{1}{2} [f(n) + f(N)] + \sum_{n=2}^{\infty} \frac{B_n}{n!} \left[ \frac{d^{n-1} f}{d x^{n-1}} \bigg|_{x=N} - \frac{d^{n-1} f}{d x^{n-1}} \bigg|_{x=n} \right].
\]  

(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 \(n \gg 1\).

\[
\Gamma(n + 1) = n!,
\]  

(26)
\[
\ln \left( \Gamma(n+1) \right) = \ln n! = \ln \left( 1 \cdot 2 \cdot 3 \cdots \cdot (n-1) \cdot n \right) = \sum_{k=1}^{n} \ln k.
\] (27)

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

\[
\ln \left( \Gamma(n+1) \right) = \ln(n!) = \int_{1}^{n} \ln(x) \, dx + \frac{1}{2} \left( \ln(1) + \ln(n) \right)
\]
\[
= x \ln(x) \bigg|_{1}^{n} - \int_{1}^{n} \frac{x}{x} \, dx + \frac{1}{2} \ln(n)
\]
\[
= n \ln(n) - n + 1 + \frac{1}{2} \ln(n).
\] (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,

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

or

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

In order to find the constant in Eq. (30), we are going to use the duplication formula for Gamma function, Eq. (51). We first rewrite eq. (51) as following:

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

or

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

Let’s assume without proof that Eq. (30) that we derived for large integer \( n \) works also for any large positive argument. It is indeed a reasonable assumption – if Eq. (30) is a good approximation for both \( \Gamma(n) \) and for \( \Gamma(n+1) \), it works with the same error bound (since \( \Gamma(x) \) is monotoneous for \( x > 1 \)) in between \( n \) and \( n + 1 \). Therefore,

\[
\Gamma \left( n + \frac{1}{2} \right) = \Gamma \left( n - \frac{1}{2} + 1 \right) \approx C \left( n - \frac{1}{2} \right)^{n} e^{-n + \frac{1}{2}}.
\] (33)
For \( n \gg 1 \),
\[
\left( n - \frac{1}{2} \right)^n = n^n \left\{ \left( 1 - \frac{1}{2n} \right)^{2n} \right\}^{\frac{1}{2}} \approx n^n e^{-\frac{1}{2}}. 
\] (34)

Thus,
\[
\Gamma \left( n + \frac{1}{2} \right) \approx C n^n e^{-n}. 
\] (35)

Substituting Eq. (30), (35) into Eq. (32), we obtain:
\[
C \left( 2n \right)^{2n + \frac{1}{2}} e^{-2n} = \frac{2^{2n}}{\sqrt{\pi}} C n^{n + \frac{1}{2}} e^{-n} C n^n e^{-n}. 
\] (36)

After simplification,
\[
C = \sqrt{2\pi}. 
\] (37)

Finally,
\[
\Gamma (n + 1) = n! = \sqrt{2\pi n \left( \frac{n}{e} \right)^n} = \sqrt{2\pi n^{n + \frac{1}{2}} e^{-n}}. 
\] (38)

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

Example 1. Let's consider the following sum:

\[ S(\alpha, k) = \sum_{n=-\infty}^{\infty} e^{-\alpha(n^2)^k}, \quad \alpha > 0, \ k > 0. \]  \hspace{1cm} (39)

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

\[ S(\alpha, k) \approx \int_{-\infty}^{\infty} e^{-\alpha(x^2)^k} \, dx = \int_{0}^{\infty} e^{-\alpha x^2} \, dx. \]  \hspace{1cm} (40)

Introduction of a new integration variable,

\[ u = \alpha x^2k \rightarrow x = \left(\frac{u}{\alpha}\right)^{\frac{1}{2k}} \rightarrow dx = \frac{1}{2k} \alpha^{-\frac{1}{2k}} u^{-\frac{1}{2k}-1} \, du, \]  \hspace{1cm} (41)

transforms the integral as following:

\[ \frac{1}{2k} \alpha^{-\frac{1}{2k}} \int_{0}^{\infty} e^{-u} u^{-\frac{1}{2k}-\frac{1}{2k}} \, du = \frac{\alpha^{-\frac{1}{2k}}}{k} \Gamma\left(\frac{1}{2k}\right), \]  \hspace{1cm} (42)

so that

\[ S(\alpha, k) \approx \frac{\alpha^{-\frac{1}{2k}}}{k} \Gamma\left(\frac{1}{2k}\right). \]  \hspace{1cm} (43)

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

Example 2. Let's consider the following sum:

\[ S(\alpha) = \sum_{n=0}^{\infty} (2n+1) e^{-\alpha n(n+1)}. \]  \hspace{1cm} (44)

As in the example above, the case of small \( \alpha, \alpha \ll 1, \) is most difficult for a numerical summation, since many terms need to be added in the sum Eq. (44). Small \( \alpha \) is where the Euler-Maclaurin approximation works the best.
Figure 2: Euler-Maclaurin approximation Eq. (43), dashed line, compared with numerical value of the sum $S(\alpha, 1) = \sum_{n=-\infty}^{\infty} e^{-\alpha n^2}$, solid line.

Figure 3: Euler-Maclaurin approximation Eq. (43), dashed line, compared with numerical value of the sum $S(\alpha, 2) = \sum_{n=-\infty}^{\infty} e^{-\alpha n^4}$, solid line.
The integral term of the Euler-Maclaurin approximation,

\[ S(\alpha) \approx \int_0^\infty (2x+1)e^{-\alpha x(x+1)} \, dx = \int_0^\infty e^{-\alpha x(x+1)} \, d\left[x(x+1)\right]. \]  

(45)

Introduction of a new integration variable,

\[ u = x(x+1), \quad 0 \leq u < \infty, \]  

(46)
transforms the integral as following:

\[ S(\alpha) = \int_0^\infty e^{-\alpha u} \, du = \frac{1}{\alpha}. \]  

(47)

The approximation Eq. (47) is compared with the results of numerical calculations of the sum Eq. (44) in Fig. 4.

Figure 4: Euler-Maclaurin approximation Eq. (47), dashed line, compared with numerical value of the sum \( S(\alpha) = \sum_{n=0}^{\infty} (2n+1)e^{-\alpha n(n+1)} \), solid line.

Example 3. 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).
Let’s consider the following sum:

\[ S_3 \equiv \sum_{k=1}^{n} k^3. \]  

(48)

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

\[
S_3 = \int_{1}^{n} x^3 \, dx + \frac{1}{2} \left( n^3 + 1 \right) + \frac{B_2}{2} \left( 3n^2 - 3 \right) + \frac{B_4}{4!} (6 - 6) \\
= \frac{1}{4} (n^4 - 1) + \frac{1}{2} (n^3 + 1) + \frac{1}{4} (n^2 - 1),
\]

(49)

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

\[ S_3 = \frac{1}{4} n^2(n + 1)^2, \]

(50)

which is indeed the correct result.

**Appendix A. Duplication formula for Gamma function**

The duplication formula for the Gamma function is

\[
\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}} \Gamma(z) \Gamma(z + \frac{1}{2})
\]

(51)

It is also called the Legendre duplication formula.

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

\[
B(z, z) = \int_{0}^{1} x^{z-1} (1-x)^{z-1} \, dx.
\]

(52)

Let’s change the integration variable to \( t \), \( x = \frac{1-t}{2} \), so that \(-1 \leq t \leq 1\) and \( dx = \frac{1}{2} \, dt \). This transforms Eq. (52) into

\[
B(z, z) = 2^{2-2z} \frac{1}{2} \int_{-1}^{1} (1-t)^{z-1} (1+t)^{z-1} \, dt = 2^{2-2z} \int_{0}^{1} (1-t^2)^{z-1} \, dt.
\]

(53)
Changing the integration variable in the last integral to $u = t^2$, so that $0 \leq u \leq 1$ and $dt = \frac{1}{2}u^{-\frac{3}{2}}$, we transform the integral to

$$B(z, z) = 2^{1-2z} \int_0^1 u^{-\frac{1}{2}} (1-u)^{z-1} du = 2^{1-2z} B\left(\frac{1}{2}, z\right),$$

i.e.

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

In terms of Gamma function,

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

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

so that

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

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

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

which is the duplication formula.

References

