EULER-MACLAURIN SUMMATION FORMULA

LECTURE NOTES, SPRING SEMESTER 2017

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

Last modified: May 19, 2017

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. 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):

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

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

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

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:

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

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

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

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:

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

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:

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

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. (51). We first rewrite eq. (51) as following:

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

or

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

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,

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

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:

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

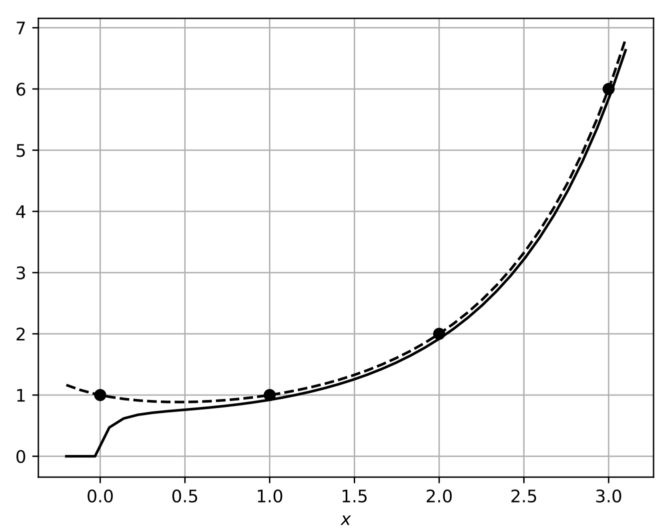
After simplification,

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

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:

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

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.

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

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.

Example 2. Lets consider the following sum:

$$S(\alpha) = \sum_{n=0}^{\infty}(2n+1)\,e^{-\alpha n(n+1)}. \tag{44}$$

As in the example above, 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. (44). Small α is where the Euler-Maclaurin approximation works the best.

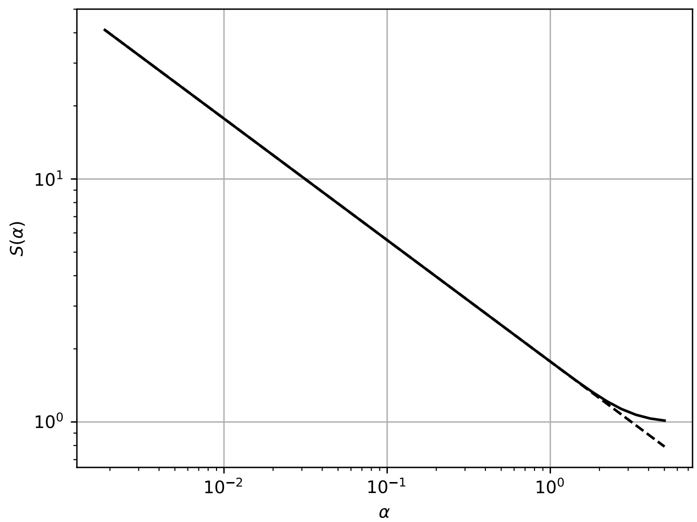


Figure 2: Euler-Maclaurin approximation Eq. (43), dashed line, compared with numerical value of the sum $S(\alpha, 1) = \sum_{n=-\infty}^{\infty} e^{-\alpha n^2}$, solid line.

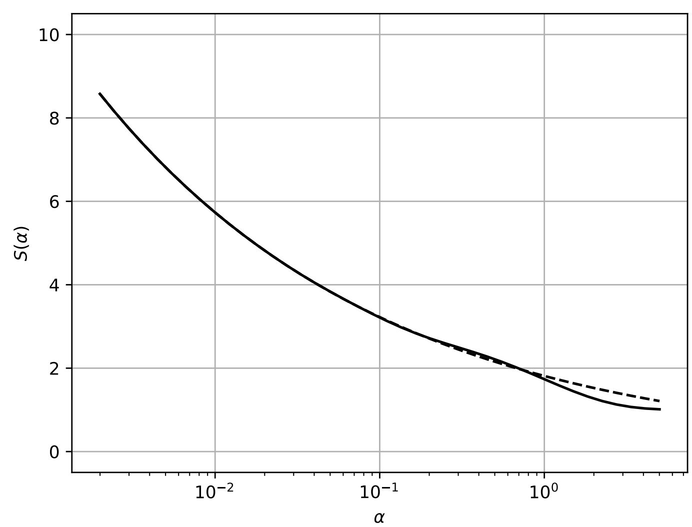


Figure 3: Euler-Maclaurin approximation Eq. (43), dashed line, compared with numerical value of the sum $S(\alpha, 2) = \sum_{n=-\infty}^{\infty} e^{-\alpha n^4}$, solid line.

The integral term of the Euler-Maclaurin approximation,

$$S(\alpha) \approx \int_0^\infty (2x+1)\, e^{-\alpha x(x+1)}\, \mathrm{d}x = \int_0^\infty e^{-\alpha x(x+1)}\, \mathrm{d}\Big[x(x+1)\Big]. \tag{45}$$

Introduction of a new integration variable,

$$u = x(x+1), \quad 0 \le u < \infty, \tag{46}$$

transforms the integral as following:

$$S(\alpha) = \int_0^\infty e^{-\alpha u}\, \mathrm{d}u = \frac{1}{\alpha}. \tag{47}$$

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

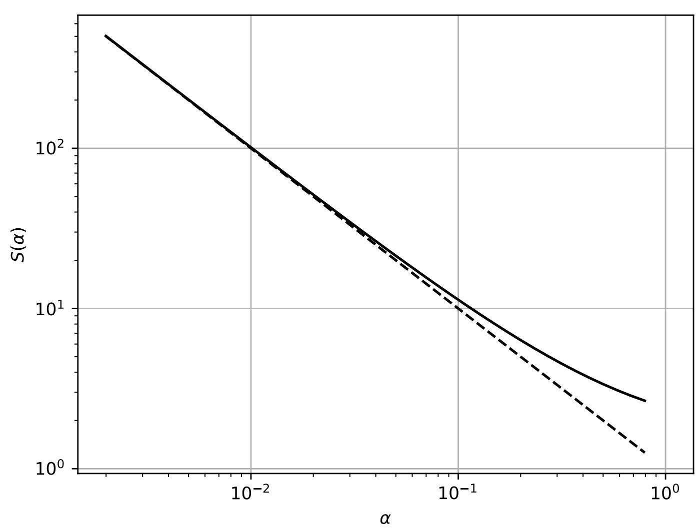


Figure 4: Euler-Maclaurin approximation Eq. (47), dashed line, compared with numerical value of the sum $S(\alpha) = \sum_{n=0}^{\infty}(2n+1)\, e^{-\alpha n(n+1)}$, solid line.

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:

$$S_3 \equiv \sum_{k=1}^{n} k^3. \tag{48}$$

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

$$\begin{aligned} S_3 &= \int_1^n x^3\,\mathrm{d}x + \frac{1}{2}\left(n^3+1\right) + \frac{B_2}{2}\left(3n^2-3\right) + \frac{B_4}{4!}(6-6) \\ &= \frac{1}{4}\left(n^4-1\right) + \frac{1}{2}\left(n^3+1\right) + \frac{1}{4}\left(n^2-1\right), \end{aligned} \tag{49}$$

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

$$S_3 = \frac{1}{4}n^2(n+1)^2, \tag{50}$$

which is indeed the correct result.

Appendix A. Duplication formula for Gamma function

The duplication formula for the Gamma function is

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}}\Gamma(z)\,\Gamma\left(z+\frac{1}{2}\right) \tag{51}$$

It is also called the Legendre duplication formula.

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

$$B(z,z) = \int_0^1 x^{z-1}(1-x)^{z-1}\mathrm{d}x. \tag{52}$$

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. (52) into

$$B(z,z) = 2^{2-2z}\frac{1}{2}\int_{-1}^{1}(1-t)^{z-1}(1+t)^{z-1}\mathrm{d}t = 2^{2-2z}\int_0^1 (1-t^2)^{z-1}\mathrm{d}t. \tag{53}$$

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

$$B(z,z) = 2^{1-2z}\int_0^1 u^{-\frac{1}{2}}(1-u)^{z-1}\,\mathrm{d}u = 2^{1-2z}B\left(\frac{1}{2},z\right), \tag{54}$$

i.e.

$$B(z,z) = 2^{1-2z}B\left(\frac{1}{2},z\right). \tag{55}$$

In terms of Gamma function,

$$B(z,z) = \frac{\Gamma(z)\Gamma(z)}{\Gamma(2z)}, \tag{56}$$

$$B\left(\frac{1}{2},z\right) = \frac{\Gamma\left(\frac{1}{2}\right)\Gamma(z)}{\Gamma\left(z+\frac{1}{2}\right)}, \tag{57}$$

so that

$$\frac{\Gamma(z)\Gamma(z)}{\Gamma(2z)} = 2^{1-2z}\frac{\Gamma\left(\frac{1}{2}\right)\Gamma(z)}{\Gamma\left(z+\frac{1}{2}\right)}. \tag{58}$$

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

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}}\Gamma(z)\Gamma\left(z+\frac{1}{2}\right), \tag{59}$$

which is the duplication formula.

References

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

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

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