4.3. Euler-Maclaurin Formula

On the contents of the lecture. From this lecture we will learn how Euler managed to calculate eighteen digit places of the sum $\sum_{k=0}^{\infty} \frac{1}{k^2}$.

Symbolic derivation. Taylor expansion of a function f at point x gives

$$f(x+1) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x)}{k!}.$$

Hence

$$\delta f(x) = \sum_{k=1}^{\infty} \frac{\mathbf{D}^k f(x)}{k!},$$

where $\mathbf{D}$ is the operation of differentiation. One expresses this equality symbolically as

$$\delta = \exp \mathbf{D} - \mathbf{1}. \tag{4.3.1}$$

We are searching for F such that $F(n) = \sum_{k=1}^{n-1} f(k)$ for all n. Then $\delta F(x) = f(x)$, or symbolically $F = \delta^{-1} f$. So we have to invert the operation of the difference. From (4.3.1), the inversion is given formally by the formula $(\exp \mathbf{D} - \mathbf{1})^{-1}$. This function has a singularity at 0 and cannot be expanded into a power series in $\mathbf{D}$. However we know the expansion

$$\frac{t}{\exp t - 1} = \sum_{k=0}^{\infty} \frac{B_k}{k!} t^k.$$

This allows us to give a symbolic solution of our problem in the form

$$\delta^{-1} = \mathbf{D}^{-1} \frac{\mathbf{D}}{\exp \mathbf{D} - \mathbf{1}} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathbf{D}^{k-1} = \mathbf{D}^{-1} - \frac{1}{2}\mathbf{1} + \sum_{k=1}^{\infty} \frac{B_{2k}}{2k!} \mathbf{D}^{2k-1}.$$

Here we take into account that $B_0 = 1$, $B_1 = -\frac{1}{2}$ and $B_{2k+1} = 0$ for $k > 0$. Since $\sum_{k=1}^{n-1} f(k) = F(n) - F(1)$, the latter symbolic formula gives the following summation formula:

$$\sum_{k=1}^{n-1} f(k) = \int_1^n f(x)\,dx - \frac{f(n) - f(1)}{2} + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!} (f^{(2k-1)}(n) - f^{(2k-1)}(1)). \tag{4.3.2}$$

For $f(x) = x^m$ this formula gives the Bernoulli polynomial ϕ_{m+1}.

Euler's estimate. Euler applied this formula to $f(x) = \frac{1}{(x+9)^2}$ and estimated the sum $\sum_{k=10}^{\infty} \frac{1}{k^2}$. In this case the k-th derivative of $\frac{1}{(x+9)^2}$ at 1 has absolute value $\frac{(k+1)!}{10^{k+2}}$. Hence the module of the k-th term of the summation formula does not exceed $\frac{B_k}{k10^{k+2}}$. For an accuracy of eighteen digit places it is sufficient to sum up the first fourteen terms of the series, only eight of them do not vanish. Euler conjectured, and we will prove, that the value of error does not exceed of the value of the first rejected term, which is $\frac{B_{16}}{16 \cdot 10^{18}}$. Since $B_{16} = -\frac{3617}{510}$ this gives the promised accuracy.

B_1	B_2	B_4	B_6	B_8	B_{10}	B_{12}	B_{14}	B_{16}	B_{18}	B_{20}
$-\frac{1}{2}$	$\frac{1}{6}$	$-\frac{1}{30}$	$\frac{1}{42}$	$-\frac{1}{30}$	$\frac{5}{66}$	$-\frac{691}{2730}$	$\frac{7}{6}$	$-\frac{3617}{510}$	$\frac{43867}{798}$	$-\frac{174611}{330}$

FIGURE 4.3.1. Bernoulli numbers

We see from the table (Figure 4.3.1) that increasing of the number of considered terms does not improve accuracy noticeably.

Summation formula with remainder. In this lecture we assume that all functions under consideration are differentiable as many times as needed.

LEMMA 4.3.1. *For any function $f(x)$ on $[0,1]$ one has*

$$\frac{1}{2}(f(1)+f(0)) = \int_0^1 f(x)\,dx - \int_0^1 f'(x)B_1(x)\,dx.$$

PROOF. Recall that $B_1(x) = x - \frac{1}{2}$, hence $\int_0^1 f'(x)B_1(x)\,dx = \int_0^1 (x-\frac{1}{2})\,df(x)$. Now, integration by parts gives

$$\int_0^1 (x-\frac{1}{2})\,df(x) = \frac{1}{2}(f(1)+f(0)) - \int_0^1 f(x)\,dx.$$

□

Consider the *periodic Bernoulli polynomials* $B_m\{x\} = B_m(x-[x])$. Then $B'_m\{x\} = mB_{m-1}\{x\}$ for non integer x.

Let us denote by $\sum_m^n a_k$ the sum $\frac{1}{2}a_m + \sum_{k=m+1}^{n-1} a_k + \frac{1}{2}a_n$.

LEMMA 4.3.2. *For any natural p, q and any function $f(x)$ one has*

$$\sum_p^q f(k) = \int_p^q f(x)\,dx - \int_p^q f'(x)B_1\{x\}\,dx.$$

PROOF. Applying Lemma 4.3.1 to $f(x+k)$ one gets

$$\begin{aligned}\frac{1}{2}(f(k+1)+f(k)) &= \int_0^1 f(x+k)\,dx + \int_0^1 f'(x+k)B_1(x)\,dx\\ &= \int_k^{k+1} f(x)\,dx + \int_k^{k+1} f'(x)B_1\{x\}\,dx.\end{aligned}$$

Summing up these equalities for k from p to q, one proves the lemma. □

LEMMA 4.3.3. *For $m>0$ and a function f one has*

$$\int_p^q f(x)B_m\{x\}\,dx = \frac{B_{m+1}}{m+1}(f(q)-f(p)) - \int_p^q f'(x)B_{m+1}\{x\}\,dx. \tag{4.3.3}$$

PROOF. Since $B_m\{x\}dx = d\frac{B_{m+1}\{x\}}{m+1}$ and $B_{m+1}\{k\} = B_{m+1}$ for any natural k, the formula (4.3.3) is obtained by a simple integration by parts. □

THEOREM 4.3.4. *For any function f and natural numbers n and m one has:*

$$\sum_1^n f(k) = \int_1^n f(x)\,dx + \sum_{k=1}^{m-1} \frac{B_{k+1}}{(k+1)!}\Big(f^{(k)}(n) - f^{(k)}(1)\Big) + \frac{(-1)^{m+1}}{m!}\int_1^n f^{(m)}(x) B_m\{x\}\,dx. \tag{4.3.4}$$

PROOF. The proof is by induction on m. For $m = 1$, formula (4.3.4) is just given by Lemma 4.3.2. Suppose (4.3.4) is proved for m. The *remainder*

$$\frac{(-1)^{m+1}}{m!}\int_1^n f^{(m)}(x) B_m\{x\}\,dx$$

can be transformed by virtue of Lemma 4.3.3 into

$$\frac{(-1)^{m+1}B_{m+1}}{(m+1)!}(f^{(m)}(n) - f^{(m)}(1)) + \frac{(-1)^{m+2}}{(m+1)!}\int_1^n B_{m+1}\{x\} f^{(m+1)}(x)\,dx.$$

Since odd Bernoulli numbers vanish, $(-1)^{m+1}B_{m+1} = B_{m+1}$ for $m > 0$. □

Estimation of the remainder. For $m = \infty$, (4.3.4) turns into (4.3.2). Denote

$$R_m = \frac{(-1)^{m+1}}{m!}\int_1^n f^{(m)}(x) B_m\{x\}\,dx.$$

This is the so-called *remainder* of Euler-Maclaurin formula.

LEMMA 4.3.5. *$R_{2m} = R_{2m+1}$ for any $m > 1$.*

PROOF. Because $B_{2m+1} = 0$, the only thing which changes in (4.3.4) when one passes from $2m$ to $2m+1$ is the remainder. Hence its value does not change either. □

LEMMA 4.3.6. *If $f(x)$ is monotone on $[0, 1]$ then*

$$\operatorname{sgn}\int_0^1 f(x) B_{2m+1}(x)\,dx = \operatorname{sgn}(f(1) - f(0)) \operatorname{sgn} B_{2m}.$$

PROOF. Since $B_{2m+1}(x) = -B_{2m+1}(1-x)$, the change $x \to 1-x$ transforms the integral $\int_{0.5}^1 f(x) B_{2m+1}(x)\,dx$ to $-\int_0^{0.5} f(1-x) B_{2m+1}(x)\,dx$:

$$\begin{aligned}\int_0^1 f(x) B_{2m+1}(x)\,dx &= \int_0^{0.5} f(x) B_{2m+1}(x)\,dx + \int_{0.5}^1 f(x) B_{2m+1}(x)\,dx \\ &= \int_0^{0.5} (f(x) - f(1-x)) B_{2m+1}(x)\,dx.\end{aligned}$$

$B_{2m+1}(x)$ is equal to 0 at the end-points of $[0, 0.5]$ and has constant sign on $(0, 0.5)$, hence its sign on the interval coincides with the sign of its derivative at 0, that is, it is equal to $\operatorname{sgn} B_{2m}$. The difference $f(x) - f(1-x)$ also has constant sign as $x < 1-x$ on $(0, 0.5)$ and its sign is $\operatorname{sgn}(f(1) - f(0))$. Hence the integrand has constant sign. Consequently the integral itself has the same sign as the integrand has. □

LEMMA 4.3.7. *If $f^{(2m+1)}(x)$ and $f^{(2m+3)}(x)$ are comonotone for $x \geq 1$ then*

$$R_{2m} = \theta_m \frac{B_{2m+2}}{(2m+2)!}(f^{(2m+1)}(n) - f^{(2m+1)}(1)), \quad 0 \leq \theta_m \leq 1.$$

PROOF. The signs of R_{2m+1} and R_{2m+3} are opposite. Indeed, by Lemma 4.2.5 $\operatorname{sgn} B_{2m} = -\operatorname{sgn} B_{2m+2}$, and $\operatorname{sgn}(f^{(2m+1)}(n) - f^{(2m+1)}(1)) = \operatorname{sgn}(f^{(2m+3)}(n) - f^{(2m+3)}(1)$ due to the comonotonity condition. Hence $\operatorname{sgn} R_{2m+1} = -\operatorname{sgn} R_{2m+3}$ by Lemma 4.3.6.

Set

$$T_{2m+2} = \frac{B_{2m+2}}{(2m+2)!}(f^{(2m+1)}(n) - f^{(2m+1)}(1)).$$

Then $T_{2m+2} = R_{2m+1} - R_{2m+2}$. By Lemma 4.3.5, $T_{2m+2} = R_{2m+1} - R_{2m+3}$. Since R_{2m+3} and R_{2m+1} have opposite signs, it follows that $\operatorname{sgn} T_{2m+2} = \operatorname{sgn} R_{2m+1}$ and $|T_{2m+2}| \geq |R_{2m+1}|$. Hence $\theta_m = \frac{R_{2m+1}}{T_{2m+2}} = \frac{R_{2m}}{T_{2m+2}}$ belongs to $[0, 1]$. $\square$

THEOREM 4.3.8. *If $f^{(k)}$ and $f^{(k+2)}$ are comonotone for any $k > 1$, then*

$$\left|\sum_1^n f(k) - \int_1^n f(x)\,dx - \sum_{k=1}^m \frac{B_{2k}}{(2k)!}\left(f^{(2k-1)}(n) - f^{(2k-1)}(1)\right)\right| \leq \left|\frac{B_{2m+2}}{(2m+2)!}\left(f^{(2m+1)}(n) - f^{(2m+1)}(1)\right)\right|.$$

Hence the value of the error which gives the summation formula (4.3.2) with m terms has the same sign as the first rejected term, and its absolute value does not exceed the absolute value of the term.

THEOREM 4.3.9. *Suppose that $\int_1^\infty |f^{(k)}(x)|\,dx < \infty$, $\lim_{x\to\infty} f^{(k)}(x) = 0$ and $f^{(k)}$ is comonotone with $f^{(k+2)}$ for all $k \geq K$ for some K. Then there is a constant C such that for any $m > K$ for some $\theta_m \in [0, 1]$*

$$\sum_{k=1}^n f(k) = C + \frac{f(n)}{2} + \int_1^n f(x)\,dx + \sum_{k=1}^m \frac{B_{2k}}{(2k)!} f^{(2k-1)}(n) + \theta_m \frac{B_{2m+2}}{(2m+2)!} f^{(2m+1)}(n). \tag{4.3.5}$$

LEMMA 4.3.10. *Under the condition of the theorem, for any $m \geq K$,*

$$\frac{(-1)^m}{m!}\int_p^\infty f^{(m)}(x) B_m\{x\}\,dx = -\theta_m \frac{B_{2m+2}}{(2m+2)!} f^{(2m+1)}(p). \tag{4.3.6}$$

PROOF. By Lemma 4.3.7,

$$\frac{(-1)^{m+1}}{m!}\int_p^q f^{(m)}(x) B_m\{x\}\,dx = \theta_m \frac{B_{2m+2}}{(2m+2)!}(f^{(2m+1)}(q) - f^{(2m+1)}(p)).$$

To get (4.3.6), pass to the limit as q tends to infinity. $\square$

PROOF OF THEOREM 4.3.9. To get (4.3.5) we change the form of the remainder R_K for (4.3.4). Since

$$\int_1^n B_K\{x\} f^{(K)}\,dx = \int_1^\infty B_K\{x\} f^{(K)}(x)\,dx - \int_n^\infty B_K\{x\} f^{(K)}(x)\,dx,$$

applying the equality (4.3.3) to the interval $[n,\infty)$, one gets

$$-\frac{(-1)^{k+1}B_k}{k!}\int_n^\infty B_k\{x\}f^{(k)}(x)\,dx = \frac{(-1)^{k+1}B_{k+1}}{(k+1)!}f^{(k)}(n) - \frac{(-1)^{k+2}B_{k+1}}{(k+1)!}\int_n^\infty B_{k+1}\{x\}f^{(k+1)}(x)\,dx.$$

Iterating this formula one gets

$$R_K = \int_1^\infty B_K\{x\}f^{(K)}\,dx + \sum_{k=K}^m \frac{B_{k+1}}{(k+1)!}f^{(k)}(n) + \frac{(-1)^m}{m!}\int_n^\infty B_m\{x\}f^{(m)}(x)\,dx.$$

Here we take into account the equalities $(-1)^k B_k = B_k$ and $(-1)^{m+2} = (-1)^m$. Now we substitute this expression of R_K into (4.3.4) and set

$$C = (-1)^{K+1}\int_1^\infty B_K\{x\}f^{(K)}(x)\,dx - \frac{f(1)}{2} - \sum_{k=1}^{K-1}\frac{B_{k+1}}{(k+1)!}f^{(k)}(1). \tag{4.3.7}$$

□

Stirling formula. The logarithm satisfies all the conditions of Theorem 4.3.9 with $K=2$. Its k-th derivative at n is equal to $\frac{(-1)^{k+1}(k-1)!}{n^k}$. Thus (4.3.5) for the logarithm turns into

$$\sum_{k=1}^n \ln k = n\ln n - n + \sigma + \frac{\ln n}{2} + \sum_{k=1}^m \frac{B_{2k}}{2k(2k-1)n^{2k-1}} + \frac{\theta_m B_{2m+2}}{(2m+2)(2m+1)n^{2k-1}}.$$

By (4.3.7), the constant is

$$\sigma = \int_1^\infty \frac{B_2\{x\}}{x^2}\,dx - \frac{B_2}{2}.$$

But we already know this constant as $\sigma = \frac{1}{2}\ln 2\pi$. For $m=0$, the above formula gives the most common form of Stirling formula:

$$n! = \sqrt{2\pi n}\,n^n e^{-n+\frac{\Theta}{12n}}.$$

Problems.

1. Write the Euler-Maclaurin series telescoping $\frac{1}{x}$.
2. Prove the uniqueness of the constant in Euler-Maclaurin formula.
3. Calculate ten digit places of $\sum_{k=1}^\infty \frac{1}{n^3}$.
4. Calculate eight digit places of $\sum_{k=1}^{1000000} \frac{1}{k}$.
5. Evaluate $\ln 1000!$ with accuracy 10^{-4}.