

Euler–Maclaurin summation and Stirling’s formula

We used the approximation

$$n! = \sqrt{2\pi} n^{n+1/2} e^{-n+\theta(n)/(12n)}$$

where $0 \leq \theta(n) \leq 1$ in understanding the behavior of the Minkowski constant. There are many proofs of this. We derive it here by proving the Euler–Maclaurin summation formula, which is hardly any more difficult than just Stirling’s result alone.

The power of integration by parts

Recall that for u, v having continuous derivatives $\int uv' dt = uv - \int vu' dt$. We can iterate this if u has higher derivatives by choosing antiderivatives of v , exploiting that they are only determined up to a constant.

Let $f(x)$ be continuously differentiable on $[0, 1]$. Compute $\int_0^1 f(x) dx$ by taking $u = f, v' = 1, v = x - 1/2$ so that $\int_0^1 v(x) dx = 0$. Then $\int_0^1 f(x) dx = [f(x)(x - 1/2)]_0^1 - \int_0^1 f'(x)(x - 1/2) dx$. This gives the trapezoidal rule with error:

$$\int_0^1 f(x) dx = (f(1) + f(0))/2 - \int_0^1 f'(x)(x - 1/2) dx$$

The error can be transformed by another integration by parts $u = f', v = x^2/2 - x/2$ to give $\int_0^1 f''(x)(x^2/2 - x/2) dx$ and the mean value theorem for integrals expresses this as $-f''(\mu)/12$ for some $\mu \in [0, 1]$. If we divide an interval $[a, b]$ into n intervals of length $h = (b - a)/n$ and apply our result to $f(t) = g(a + jh + th)$ we compute that $\int_{a+jh}^{a+(j+1)h} g(x) dx = \int_0^1 f(t)h dt = h(g(a + jh) + g(a + jh + h))/2 + h^3 \int_{a+jh}^{a+jh+h} g''(x)((x - a - jh)/h)^2/2 - (x - a - jh)/h)/2 dx$ and adding together we get the composite trapezoidal rule

$$\int_a^b g(x) dx = h(g(a)/2 + g(a + h) + \dots + g(a + (n - 1)h) + g(b)/2) + nh^3 f''(\mu)$$

If instead we choose $v = x^2/2 - x/2 + 1/12$ so that $\int_0^1 v = 0$ in the second integration by parts we get

$$\int_0^1 f(x) dx = (f(1) + f(0))/2 - (f'(1) - f'(0))/12 + \int_0^1 f''(x)(x^2/2 - x/2 + 1/12) dx$$

This is the Hermite integration formula (the same as integrating the Hermite interpolation polynomial of $f(x)$). As before we can integrate by parts in the remainder to get $[(x^3/6 - x^2/4 + x/12)f''(x)]_0^1 - \int_0^1 f'''(x)(x^3/6 - x^2/4 + x/12) dx$ and then once more using the antiderivative $x^4/24 - x^3/12 + x^2/24 = x^2(x-1)^2/24$ to get the error term $\int_0^1 f''''(x)x^2(x-1)^2/24 dx$. As above this gives the composite Hermite rule

$$\int_a^b g(x) dx = h(g(a)/2 + g(a+h) + \dots + g(b)/2) - h^2(g'(b) - g'(a))/12 + R_4$$

with remainder

$$R_4 = h^4/24 \int_a^b g''''(x)(\{(x-a)/h\}^2(\{(x-a)/h\} - 1)^2 dx$$

where $\{\}$ denotes the fractional part. By the mean value theorem this shows that the remainder is $R_4 = g''''(\mu)/24(1/30)nh^5$ for some $\mu \in [a, b]$.

Application to Stirling's formula

Take $g(x) = \log(x)$, $a = 1$, $b = N$, $h = 1$ in the composite Hermite rule above to get

$$N \log(N) - N + 1 = \log(2) + \dots \log(N-1) + \log(N)/2 - (1/N - 1)/12 + R(N)$$

with

$$R(N) = \int_1^N (-1/x^2)(\{x\}^2/2 - \{x\}/2 + 1/12) dx = \int_1^N -1/(4x^4)(\{x-1\})^2(\{x-1\} - 1)^2 dx.$$

Since the latter integral has negative integrand, $R(N+1) < R(N)$. We write $R(N) = \int_1^\infty (-1/x^2)(\{x\}^2/2 - \{x\}/2 + 1/12) dx - \int_N^\infty (-1/x^2)(\{x\}^2/2 - \{x\}/2 + 1/12) dx$. Set $C = 1 - 1/12 + \int_1^\infty (1/x^2)(\{x\}^2/2 - \{x\}/2 + 1/12) dx$. We then have

$$\log N! = (N + 1/2) \log N - N + 1 + (1/12N) + C - \int_N^\infty (1/x^2)(\{x\}^2/2 - x/2 + 1/12) dx$$

The final integral is at most $1/(12N)$, and is positive since it is the sum of positive terms $R(m) - R(m+1)$. We have

$$\log N! = C + (N + 1/2) \log N - N + \theta(N)/(12N)$$

with $0 < \theta(N) < 1$. The case $N = 1$ shows that $C = 1 - \theta(1)/12$ so that $1 > C > 11/12$. In fact, $C = \log(\sqrt{2\pi})$, as can be seen by using the Wallis formula

$$\sqrt{\pi/2} = \lim_{n \rightarrow \infty} \frac{(2^n n!)^2}{(2n)! \sqrt{2n}}$$

and the Stirling formula above to get that $\log(\pi) = C - \log 2$

Euler–Maclaurin summation formula

We can extend the trapezoidal and Hermite integration formulae by defining polynomials $B_k(x)$ which satisfy $B_0(x) = 1$ and for $k > 0$, $B_k(x)' = kB_{k-1}(x)$, $\int_0^1 B_k(x) dx = 0$. The polynomials $B_1(x) = x - 1/2$, $B_2(x) = x^2 - x + 1/6$, $B_3(x) = x^3 - (3/2)x^2 + x/2$, $B_4(x) = x^4 - 2x^3 + x^2 - 1/30$ appeared in the paragraphs above. We set $B_k = B_k(0)$. Computing the integral $0 = \int_0^1 B_{k-1}(x) dx = [B_k(x)/k]_0^1$ for $k > 1$ gives $B_k(1) = B_k(0)$. Further, the polynomials $C_k(x) = (-1)^k B_k(1-x)$ satisfy $C_0(x) = 1$, $C_k(x)' = kC_{k-1}(x)$, $\int_0^1 C_k(x) dx = 0$ so that $B_k(x) = (-1)^k B_k(1-x)$ so $B_k = (-1)^k B_k(1)$ and for odd $k > 1$ we have $B_k = 0$. The generating series for the Bernoulli polynomials $B_k(x)$ is $F(x, t) = \sum B_k(x)t^k/k!$. The definition shows that $F_x(x, t) = tF(x, t)$ so that $F(x, t) = F(0, t)e^{tx}$. Integrating both sides of this equation for $x \in [0, 1]$ and using that $B_k(x)$ has average 0 for $k > 0$ gives that $1 = F(0, t)(e^t - 1)/t$ or $F(x, t) = te^{xt}/(e^t - 1) = \sum B_k(x)t^k/k!$ which makes transparent many properties of the Bernoulli numbers B_k .

Continued integration by parts assuming f has m continuous derivatives yields that $\int_0^1 f(x) dx = f(0)/2 + f(1)/2 - \int_0^1 f^{(1)}(x)B_1(x)/1! dx$

$$\begin{aligned} &= f(0)/2 + f(1)/2 - [f(x)B_2(x)/2]_0^1 + \int_0^1 f^{(2)}(x)B_2(x)/2! dx \\ &= f(0)/2 + f(1)/2 - [f(x)B_2(x)/2]_0^1 - [f(x)B_3(x)/3!]_0^1 - \int_0^1 f^{(3)}(x)B_3(x)/3! dx \\ &= f(0)/2 + f(1)/2 - \sum_{k=2}^m [f^{(k-1)}(x)B_k(x)/k!]_0^1 + (-1)^m \int_0^1 f^{(m)}(x)B_m(x)/m! dx \end{aligned}$$

It is convenient to require that for $B_k(1) - B_k(0) = \int k B_{k-1}(x) dx = 0$ for $k \geq 2$ and to define $B_k = B_k(0)$ so that the formula simplifies to

$$\int_0^1 f(x) dx = f(0)/2 + f(1)/2 - \sum_{k=2}^m [f^{(k-1)}(x)B_k/k!]_0^1 + (-1)^m \int_0^1 f^{(m)}(x)B_m(x)/m! dx$$

Further, the polynomials $B_k(x)$ are determined by $B_0(x) = 1$, $B_k(x) = kB_{k-1}(x)$, and for $k > 0$, $\int_0^1 B_k(x) dx = 0$. We have that the Bernoulli polynomial $B_k(x)$ is expressible in terms of the Bernoulli numbers $B_k = B_k(0)$ as

$$B_k(x) = \sum_{j=0}^k \binom{k}{j} B_j x^{k-j}$$

When f has m continuous derivatives on $[M, N]$ we can add the previous formulae for functions $f(x+j)$, $j = M \dots N-1$ to obtain the Euler–Maclaurin summation formula:

$$\int_M^N f(x) dx = f(N)/2 + \sum_{k=M+1}^{N-1} f(k) + f(M)/2 - \sum_{k=2}^m [f^{(k-1)}(x)]_M^N B_k/k! + R_m$$

where

$$R_m = (-1)^m \int_M^N f^{(m)}(x) B_m(\{x\})/m! dx$$

The remainder term R_m can be rewritten by further integration by parts when $m \geq 2$. The version above is sufficient for many purposes.

Solving for the sum of function values gives that

$$f(N)/2 + \sum_{k=M+1}^{N-1} f(k) + f(M)/2 = \int_M^N f(x) dx + \sum_{k=2}^m [f^{(k-1)}(x)]_M^N B_k/k! - R_m$$

Taking $B_1(x) = x - 1/2$, $B_1 = -1/2$ we can rewrite this as

$$\sum_{j=M}^{N-1} f(j) = \int_M^N f(x) dx + \sum_{k=1}^m [f^{(k-1)}(x)]_M^N B_k/k! - R_m$$

Application 0: Let $g(x)$ be defined on the interval $[a, b]$ and divide the interval into N subintervals of equal length $h = (b - a)/n$.

Let $M = 0$, $f(x) = g(a + xh)$. Taking the first formula when $m = 1$ gives the trapezoidal rule with error

$$\int_0^N g(a + xh) dx = g(a)/2 + g(a+h) + \cdots + g(b-h) + g(b)/2 + \int_0^N hg(a + xh)((x)B_1(\{x\})) dx$$

Substituting $u = a + hx$ gives the usual form

$$\int_a^b g(u) du = (1/h)(g(a)/2 + g(a+h) + \cdots + g(b-h) + g(b)/2) + \int_a^b g(u)((u-a)/h)B_1(\{(u-a)/h\}) du$$

Application 1: Let l be a positive integer and take $f(x) = x^l$. The formula above with $M = 0$, $m = l + 1$ gives

$$(l+1) \sum_{j=0}^{N-1} j^l = N^{l+1} + \sum_{k=1}^l B_k \binom{l+1}{k} N^{l+1-k} = B_{l+1}(N) - B_{l+1}$$

Application 2: Fix a positive integer period r and integer $j = 0, \dots, r-1$ and let $f(x) = (rx + j)^{-s}$. When the real part of s exceeds 1 the sum $L(f, s) = \sum_{n=1}^{\infty} f(n)$ converges and by taking the limit as $N \rightarrow \infty$ in the Euler–Maclaurin formula with $M = 1$ equals

$$(r + j)^{-s+1}/(r(s-1)) - \sum_{k=1}^m f^{(k-1)}(1)B_k/k! + (-1)^{m+1} \int_1^{\infty} f^{(m)}(x)B_m(\{x\})/m! dx.$$

Since $f^{(k)}(x) = r^k(-s)(-s-1)\cdots(-s-k+1)(rx+j)^{-s-k}$ the expression on the right above is defined for s with real part greater than $1-m$, so it defines a continuation for $L(f, s) = \sum f(n)/n^s$ to s in that range, hence to all complex numbers since m can be arbitrarily large. Further, for the integer $s = 1-m$ we have $f^{(m)}(x) = 0$ so that $L(f, 1-m) = (r+j)^{-m}/(-rm) - \sum_{k=1}^m r^{k-1}(m-1)(m-2)\cdots(m-k)(r+j)^{m-k}B_k/k!$ is the rational number $(-1/mr)B_m(1+j/r)$. For example when $r = 1, j = 0$ we obtain that $L(f, s)$ is the zeta function $\zeta(s) = \sum n^{-s}$ and that $\zeta(1-m) = -B_m(1)/m$, so that $\zeta(0) = -1/2$ and for $m > 1$, $\zeta(1-m) = -B_m/m$.

For any periodic function $\chi(x)$ on the nonnegative integers with $\chi(x+r) = \chi(x)$ the function $L(\chi, s) = \sum_{n=1}^{\infty} \chi(n)/n^s$ is a finite linear combination $\sum_{j=0}^{r-1} \chi(j)L(f_j, s)$ of functions analytically continued in the first paragraph. So $L(\chi, s)$ can be continued to a meromorphic function on the complex plane and has possible poles only at $s = 1$ with polar part $(\sum_{j=0}^r \chi(j))/(r(s-1))$ and takes values at negative integers in the field generated by the values of χ over the rational field. For example, this yields a closed form for the value at $s = 0$ of the continuation as $L(\chi, 0) = (-1/r) \sum_{j=0}^{r-1} \chi(j)(1/2 + j/r)$.