January 29, 2012

Euler-Maclaurin Summation Formula[1]

Suppose that f and its derivative are continuous functions on the closed interval $[a, b]$. Let

$$\psi(x) = \{x\} - \frac{1}{2},$$

where $\{x\} = x - [x]$ is the fractional part of x.

Lemma 1: If $a < b$ and $a, b \in \mathbb{Z}$, then

$$\sum_{a<n\le b} f(n) = \int_a^b \left(f(x) + \psi(x)f'(x)\right)\, dx + \frac{1}{2}\left(f(b) - f(a)\right).$$

Proof: The proof proceeds along the lines of the Abel partial summation formula.

$$\begin{aligned}
\sum_{a<n\le b} f(n) &= (b-a-1)f(b) + f(a) - \sum_{a\le n\le b-1} (n-a-1)\left(f(n+1) - f(n)\right) \\
&= (b-a-1)f(b) + f(a) - \sum_{a\le n\le b-1} (n-a-1)\int_n^{n+1} f'(t)\,dt \\
&= (b-a-1)f(b) + f(a) - \sum_{a\le n\le b-1} \int_n^{n+1} \left([t]-a-1\right) f'(t)\,dt \\
&= (b-a-1)f(b) + f(a) + (a+1)\int_a^b f'(t)\,dt - \int_a^b [t]f'(t)\,dt \\
&= bf(b) - af(a) - \int_a^b (t - \{t\})f'(t)\,dt \\
&= \int_a^b f(t)\,dt + \int_a^b \{t\}f'(t)\,dt \\
&= \int_a^b f(t)\,dt + \int_a^b \left(\{t\} - \frac{1}{2}\right) f'(t)\,dt + \frac{1}{2}(f(b) - f(a)) \\
&= \int_a^b \left(f(t) + \psi(t)f'(t)\right)\, dt + \frac{1}{2}(f(b) - f(a)).
\end{aligned}$$

We define *Bernoulli polynomials* by the following three properties[2]

$$B_0(x) = 1, \tag{1}$$

$$B_k'(x) = kB_{k-1}(x), \quad k = 1, 2, \ldots, \tag{2}$$

$$\int_0^1 B_k(x)\,dx = 0, \quad k = 1, 2, \ldots. \tag{3}$$

To determine the polynomials we introduce a generating function

$$F(t, x) = \sum_{k=0}^{\infty} B_k(x)\frac{t^k}{k!}.$$

[1] These notes follow *Analytic Number Theory* by H. Iwaniec & E. Kowalski.

[2] Property (2) defines B_k, $k \ge 1$ recursively up to a constant. The constant is fixed by property (3).

Observe

$$\frac{\partial F(t,x)}{\partial x} = \sum_{k\geq 0} B_k'(x)\frac{t^k}{k!} = \sum_{k\geq 1} kB_{k-1}(x)\frac{t^k}{k!} = t\sum_{k\geq 1} B_{k-1}(x)\frac{t^{k-1}}{(k-1)!} = tF(t,x).$$

Thus

$$F(t,x) = C(t)e^{tx} \tag{4}$$

where C is some function of t. Now by the third defining property of $B_k(x)$,

$$\int_0^1 F(t,x)\,dx = 1.$$

Integrating both sides of (4) with respect to x over the interval $[0,1]$ then implies

$$C(t) = \frac{t}{e^t - 1},$$

and hence;

$$\sum_{k\geq 0} B_k(x)\frac{t^k}{k!} = \frac{te^{tx}}{e^t - 1}.$$

Using this generating function we can find the first few Bernoulli polynomials:

$$\begin{aligned}
B_0(x) &= 1,\\
B_1(x) &= x - \frac{1}{2},\\
B_2(x) &= x^2 - x + \frac{1}{6},\\
B_3(x) &= x^3 - \frac{3}{2}x^2 + \frac{1}{2}x,\\
B_4(x) &= x^4 - 2x^3 + x^2 - \frac{1}{30},\\
B_5(x) &= x^5 - \frac{5}{2}x^4 + \frac{5}{3}x^3 - \frac{1}{6}x,\\
B_6(x) &= x^6 - 3x^5 + \frac{5}{2}x^4 - \frac{1}{2}x^2 + \frac{1}{42}.
\end{aligned}$$

The *Bernoulli numbers* are defined by

$$B_n = B_n(0),$$

that is, the value of the Bernoulli polynomial at $x = 0$. The generating function for Bernoulli numbers is clearly

$$F(t) := \sum_{n\geq 0} B_k\frac{t^k}{k!} = \frac{t}{e^t - 1}.$$

An easy calculation shows $F(-t) = F(t) + t$; and hence, $F(-t) - F(t) = t$. This last equality implies that $B_{2k+1} = 0$ for $k = 1, 2, \ldots$.

Define

$$\psi_k(x) = B_k(\{x\}) \tag{5}$$

where $\{x\}$ is the fractional part of x. Observe that $\psi(x) = \psi_1(x) = \{x\} - \frac{1}{2}$ which appears in Lemma 1. Since $\{x\}$ is periodic with period 1, so too are the functions $\psi_k(x)$ and they have generating function

$$\sum_{k\geq 0} \psi_k(x)\frac{t^k}{k!} = \frac{te^{t\,\{x\}}}{e^t - 1}$$

We now assume that f is twice continuously differentiable in $[a,b]$. We integrate by parts the term involving ψ_1 in Lemma 1. First look at

$$\int_a^{a+1} f'(x)\psi_1(x)\,dx = \int_0^1 f'(t+a)\psi_1(t+a)\,dt = \int_0^1 f'(t+a)\psi_1(t)\,dt \tag{6}$$

since ψ_1 is 1-periodic. In the interval $[0,1]$, $\psi_1(t) = B_1(t)$. Thus

$$\int_0^x \psi_1(t)\,dt = \frac{1}{2}(\psi_2(x) - B_2)$$

where we used defining property (2) of the Bernoulli polynomials. Note that $\int_0^1 \psi_1(x)\,dx = 0$ since ψ_2 is 1-periodic.

Integrating the last integral in (6) by parts gives

$$\begin{aligned}
\int_a^{a+1} f'(x)\psi_1(x)\,dx &= f'(y+a)\int_0^y \psi_1(t)\,dt\Big|_{y=0}^{y=1} - \int_0^1 f''(y+a)\int_0^y \psi_1(t)\,dt \\
&= -\int_0^1 f''(y+a)\frac{1}{2}\left(\psi_2(y) - B_2\right) \\
&= -\frac{1}{2}\int_0^1 f''(y+a)\psi_2(y)\,dy + \frac{1}{2}B_2\left(f'(a+1) - f'(a)\right) \\
&= -\frac{1}{2}\int_a^{a+1} f''(x)\psi_2(x)\,dx + \frac{1}{2}B_2\left(f'(a+1) - f'(a)\right)
\end{aligned}$$

since ψ_2 is 1-periodic. One notes that the above formula is valid over any interval $[a+n-1, a+n]$; namely,

$$\int_{a+n-1}^{a+n} f'(x)\psi_1(x)\,dx = -\frac{1}{2}\int_{a+n-1}^{a+n} f''(x)\psi_2(x)\,dx + \frac{1}{2}B_2\left(f'(a+n) - f'(a+n-1)\right),\ n = 0, 1, \ldots, b-a.$$

Summing over n we obtain

$$\int_a^b f'(x)\psi_1(x)\,dx = -\frac{1}{2}\int_a^b f''(x)\psi_2(x)\,dx + \frac{1}{2}B_2\left(f'(b) - f'(a)\right).$$

We have proved

Lemma 2: Let f be twice continuously differentiable on $[a,b]$ where $a < b$ and $a, b \in \mathbb{Z}$. Then

$$\sum_{a<n\le b} f(n) = \int_a^b \left\{ f(x) - \frac{1}{2}\psi_2(x) f''(x) \right\} dx + \sum_{\ell=1}^{2} \frac{(-1)^\ell}{\ell!}\left(f^{\ell-1}(b) - f^{\ell-1}(a)\right) B_\ell.$$

(Recall $B_1 = -\frac{1}{2}$.)

If one continues to integrate by parts one obtains the

Theorem (Euler-Maclaurin formula): Suppose f is k-times continuously differentiable on the interval $[a,b]$ with $a < b$, $a, b \in \mathbb{Z}$. Then

$$\sum_{a<n\le b} f(n) = \int_a^b \left\{ f(x) - \frac{(-1)^k}{k!}\psi_k(x) f^{(k)}(x) \right\} dx + \sum_{\ell=1}^{k} \frac{(-1)^\ell}{\ell!}\left(f^{(\ell-1)}(b) - f^{(\ell-1)}(a)\right) B_\ell.$$

Suppose f and all its derivatives go to zero as $x \to \infty$. Then we obtain by letting $b \to \infty$ (and adding $f(a)$ to both sides)

$$\boxed{\sum_{n=a}^{\infty} f(n) = \int_a^\infty f(x)\,dx + \frac{1}{2}f(a) - \sum_{\ell=2}^{k} \frac{(-1)^\ell}{\ell!} f^{(\ell-1)}(a)B_\ell - \frac{(-1)^k}{k!}\int_a^\infty f^{(k)}(x)\psi_k(x)\,dx} \tag{7}$$

Application of summation formula to the Riemann zeta-function

Let $s = \sigma + it$ where σ is the real part of s and t is the imaginary part of s. Let $\sigma > 1$ and define the Riemann zeta-function

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}, \;\; \Re(s) > 1. \tag{8}$$

The series converges absolutely and uniformly in the half-plane $\sigma = \Re(s) \geq 1 + \varepsilon$: First observe that

$$|n^{-s}| = |n^{-\sigma - it}| = n^{-\sigma} \leq n^{-1-\varepsilon}$$

Now apply the Weiestrass M-test to the series

$$\sum_{n=1}^{\infty} \frac{1}{n^{1+\varepsilon}}$$

which is convergent for all $\varepsilon > 0$. The series (8) clearly diverges at $s = 1$.

We now apply (7) with $k = 1$ to (8). Choose $f(x) = 1/x^s$. For $\Re(s) > 1$,

$$\int_1^\infty \frac{dx}{x^s} = \frac{1}{s-1}.$$

The summation formula then becomes

$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} - s\int_1^\infty \frac{1}{x^{s+1}}\,\psi_1(x)\,dx.$$

This is derived under the assumption that $\sigma > 1$. Observe that if we write

$$\zeta(s) - \frac{1}{s-1} = \frac{1}{2} - s\int_1^\infty \frac{1}{x^{s+1}}\,\psi_1(x)\,dx$$

then the right-hand side of the above equation defines a holomorphic function for $\sigma > 0$ since the integral

$$|\int_1^\infty \frac{1}{x^{s+1}}\,\psi_1(x)\,dx| \leq \int_1^\infty \frac{1}{x^{1+\sigma}}\,dx < \infty \tag{9}$$

(We used $|\psi_1(x)| \leq 1/2$.) We now use the *right-hand side* (9) to define the left-hand side of (9) for $0 < \sigma \leq 1$. The two side agree for $\sigma > 1$. This is an example of *analytic continuation*. We have made sense out of the Riemann zeta-function for $0 < \Re(s)$. We see that it has a simple pole at $s = 1$ and is holomorphic for all other points $\Re(s) > 0$.

If we apply (7) to (8) for arbitrary positive integer k we obtain after some elementary computations

$$\zeta(s) = \frac{1}{s-1} + \frac{1}{2} + \sum_{\ell=2}^{k} \frac{B_\ell}{\ell!} s(s+1)\cdots(s+\ell-2) - \frac{(-1)^k}{k!}\int_1^\infty s(s+1)\cdots(s+k-1)x^{-s-k}\psi_k(x)\,dx$$

Since ψ_k is 1-periodic and equal to the polynomial $B_k(x)$ on $[0,1)$, $\psi_k(x)$ is a bounded function on all of $\mathbb{R}$. Thus the integral on the right-hand side is convergent for all $\sigma+k>1$ and thus defines a holomorphic function for $\sigma > 1-k$. By repeating the above argument we see that we have analytically continued the Riemann zeta-function to the right-half plane $\sigma > 1-k$, for all $k = 1, 2, 3, \ldots$. For example, it now makes sense to ask for the value $\zeta'(-1)$.[3] We summarize our findings in

THEOREM: The Riemann zeta-function $\zeta(s)$ defined by (8) for $\Re(s) > 1$ can be analytically continued to $\mathbb{C} - \{1\}$ where it is holomorphic and at $s = 1$, $\zeta(s)$ has a simple pole.

[3] Before we analytically continued $\zeta(s)$ it clearly makes no sense in (8) to ask for the derivative at $s = -1$ since the series only converges for $\Re(s) > 1$. It is a fact that $\zeta'(-1) \approx -0.1654211437\ldots$.