The Euler-Maclaurin Summation Formula and Bernoulli Polynomials

Consider two different ways of applying integration by parts to $\int_0^1 f(x)dx$.

$$\int_0^1 f(x)dx = [xf(x)]_0^1 - \int_0^1 xf'(x)dx = f(1) - \int_0^1 xf'(x)dx \tag{1}$$

$$\int_0^1 f(x)dx = [(x-1/2)f(x)]_0^1 - \int_0^1 (x-1/2)f'(x)dx = \frac{f(1)+f(0)}{2} - \int_0^1 (x-1/2)f'(x)dx \tag{2}$$

The constant of integration was chosen to be 0 in (1), but $-1/2$ in (2). Which way is better? In general (2) is better. Since $\int_0^1 (x-1/2)dx = 0$, that is $x-1/2$ has zero average in $(0,1)$, it has better chance of reducing the last integral term, which is regarded as the error in estimating the given integral. We can again apply integration by parts to (2). Then the last integral will have $f''(x)$ multiplied by an integral of $x-1/2$. We can select the constant of integration in such a way that the new polynomial multiplying $f''(x)$ will have zero average in the interval. If we continue this way we will get a formula which will have a higher derivative of f in the last integral multiplying a higher degree polynomial in x. If at each step the constant of integration is chosen in such a way that the new polynomial has zero average over $(0,1)$, we will get the Euler-Maclaurin summation formula. We will also encounter polynomials related to the Bernoulli numbers, the Bernoulli Polynomials.

In the example above, integration by parts creates a sequence of polynomials in which the n-th polynomial is the integral of the $(n-1)$-th polynomial. Such sequences are best studied using the theory of **Appell Sequences**, named after the French mathematician Paul Emile Appell(1855-1930).

Appell Sequences: A sequence of polynomials $A_n(x), \quad n = 0,1,2,\ldots$ is called an Appell sequence if the following two conditions are satisfied.

$$\deg(A_n) = n, \quad n = 0,1,2,\cdots \tag{3}$$

$$A_n^{'}(x) = nA_{n-1}(x), \quad n = 1,2,3,\cdots \tag{4}$$

The most familiar Appell sequence is $1, x, x^2, x^3, \cdots$. An Appell sequence is thus a generalization of the powers of x. Because of property (4), an Appell sequence can be constructed by successive integration. It is determined completely by the constants of integration chosen at each step to satisfy additional specifications. If the constants of integration are $a_0, a_1, a_2, \ldots$, then the Appell sequence formed is seen to be $A_0(x) = a_0$, $A_1(x) = a_0x + a_1$, $A_2(x) = a_0x^2 + 2a_1x + a_2$, $A_3(x) = a_0x^3 + 3a_1x^2 + 3a_2x + a_3$, ... In general,

$$A_n(x) = \sum_{k=0}^{n} a_k \binom{n}{k} x^{n-k} \tag{5}$$

Given an Appell sequence, $A_n(x)$, $n = 0,1,2,\ldots$, the function

$$G(x,z) = \sum_{k=0}^{\infty} A_k(x)\frac{z^k}{k!} \tag{6}$$

is called its **generating function**. The generating function allows one to represent the entire sequence concisely. Since

$$\frac{\partial G(x,z)}{\partial x} = \sum_{k=0}^{\infty} A_k^{'}(x)\frac{z^k}{k!} = \sum_{k=1}^{\infty} kA_{k-1}(x)\frac{z^k}{k!} = z\sum_{k=1}^{\infty} A_{k-1}(x)\frac{z^{k-1}}{(k-1)!} = z\sum_{m=0}^{\infty} A_m(x)\frac{z^m}{m!} = zG(x,z)$$

we must have

$$G(x,z) = e^{zx}G(0,z) = e^{zx}g(z) \tag{7}$$

where $g(z) = G(0,z)$ is to be determined from other specifications. This specific form for the generating function is the main result of Appell theory.

Bernoulli Polynomials: The sequence of Bernoulli polynomials $B_n(x)$, $n = 0,1,2,\ldots$ is defined to be the Appell sequence which satisfies the additional conditions $B_0(x) = 1$, and $\int_0^1 B_n(x)dx = 0$, for $n = 1,2,3,\ldots$. So for the Bernoulli polynomials

$$B_0(x) = 1 \tag{8}$$

$$B_n^{'}(x) = nB_{n-1}(x) \tag{9}$$

$$\int_0^1 B_n(x)dx = 0, \quad n = 1,2,3,\ldots \tag{10}$$

By the theory of Appell sequences

$$\sum_{k=0}^{\infty} B_k(x)\frac{z^k}{k!} = g(z)e^{zx} \tag{11}$$

To determine $g(z)$ we integrate both sides of (11) with respect to x from 0 to 1. By property (10) integrals of all $B_n(x)$ except $B_0(x)$ on the left-hand side are zero, so the left hand side becomes 1. So,

$$1 = \int_0^1 g(z)e^{zx}dx = g(z)\frac{e^z - 1}{z}$$

Or, $g(z) = z/(e^z - 1)$. Substituting this in (11) we get

$$\frac{z}{e^z - 1}e^{zx} = \sum_{k=0}^{\infty} B_k(x)\frac{z^k}{k!} \tag{12}$$

Often this is taken as the definition of the Bernoulli polynomials, but for us this is a consequence of other requirements. It should be noted that since $z/(e^z - 1)$ generates the Bernoulli numbers, they are intimately related to the Bernoulli polynomials. Using (12) we can derive various properties of $B_n(x)$.

Properties: If we set $x = 0$ in (12) the left hand side becomes $z/(e^z - 1)$. Expanding this using the Bernoulli numbers and comparing with the right-hand side we get,

$$B_n(0) = B_n \tag{13}$$

This justifies the use of the same symbol B_n for both the polynomials and the numbers. If we set $x = 1$ in (12) we get

$$\frac{z}{e^z - 1}e^z = z + \frac{z}{e^z - 1} = z + \sum_{k=0}^{\infty} B_k\frac{z^k}{k!} = \sum_{k=0}^{\infty} B_k(1)\frac{z^k}{k!}$$

$$\Rightarrow \; B_k(1) = \begin{cases} B_k & k \neq 1; \\ B_1 + 1 = 1/2 & k = 1. \end{cases} \tag{14}$$

Since $B_k = 0$ if k is odd and not equal to 1, $B_{2k+1}(1) = 0$, for $k = 1, 2, 3, \ldots$. If we set $x = 1/2$ in (12) the left-hand side becomes $ze^{z/2}/(e^z - 1) = z/(e^{z/2} - e^{-z/2})$ which is an even function of z. This implies that $B_n(1/2)$ is 0 for all odd n.

$$B_{2k+1}(1/2) = 0, \quad k \in \mathbf{Z} \tag{15}$$

So, for odd $n > 1$, $B_n(x)$ has zeros at $x = 0$, $x = 1/2$, and $x = 1$. Does $B_n(x)$ have even/odd symmetry about $x = 1/2$? That is, is there a relationship between $B_n(1-x)$ and $B_n(x)$? $B_n(1-x)$ satisfies (8) and (10) but not (9) since $B_n^{'}(1 - x) = -nB_{n-1}(1 - x)$. To fix this problem we consider $b_n(x) = (-1)^n B_n(1 - x)$ and it satisfies all of (8), (9), and (10). So, by the definition of the Bernoulli polynomials, $(-1)^n B_n(1-x) = B_n(x)$. So we have

$$B_n(1 - x) = (-1)^n B_n(x) \tag{16}$$

$B_n(x)$ can be expressed in terms of the Bernoulli numbers by expanding both $z/(e^z - 1)$ and e^{zx} in powers of z and multiplying the two power series in (12).

$$B_n(x) = \sum_{k=0}^{n} B_k \binom{n}{k} x^{n-k} \tag{17}$$

In particular, $B_0(x) = 1$, $B_1(x) = x - 1/2$, and $B_2(x) = x^2 - x + 1/6$. If we start with $B_0(x) = 1$, and integrate repeatedly with respect to x we get a sequence of polynomials of increasing degree. If we select the integration constant at each step so that the new polynomial obtained has zero average over $(0, 1)$, we get the sequence $B_0(x)$, $B_1(x)$, $B_2(x)/2$, $B_3(x)/6$, $\ldots$, $B_n(x)/(n!)$, $\ldots$.

The Euler-Maclaurin Summation Formula: Now we integrate by parts using the Bernoulli polynomials.

$$\int_0^1 f(x)dx = \int_0^1 B_0(x)f(x)dx = [B_1(x)f(x)]_0^1 - \int_0^1 B_1(x)f'(x)dx = \frac{f(1) + f(0)}{2} - \int_0^1 B_1(x)f'(x)dx$$

$$= \frac{f(1) + f(0)}{2} - [\frac{B_2(x)f'(x)}{2!}]_0^1 + \frac{1}{2!}\int_0^1 B_2(x)f''(x)dx = \frac{f(1) + f(0)}{2} - \frac{B_2}{2!}[f'(1) - f'(0)] + \frac{1}{2!}\int_0^1 B_2(x)f''(x)dx$$

$$= \frac{f(1) + f(0)}{2} - \frac{B_2}{2!}[f'(1) - f'(0)] + \left[\frac{B_3(x)f''(x)}{3!}\right]_0^1 - \frac{1}{3!}\int_0^1 B_3(x)f'''(x)dx$$

$$= \frac{f(1)+f(0)}{2} - \frac{B_2}{2!}[f'(1)-f'(0)] - \frac{1}{3!}\int_0^1 B_3(x)f'''(x)dx$$

since $B_3(0) = B_3(1) = 0$, 3 being odd and greater than 1. Continuing in the same way we get

$$\int_0^1 f(x)dx = \frac{f(1)+f(0)}{2} - \sum_{k=1}^{n} \frac{B_{2k}}{(2k)!}[f^{(2k-1)}(1) - f^{(2k-1)}(0)] - \frac{1}{(2n+1)!}\int_0^1 B_{2n+1}(x)f^{(2n+1)}(x)dx \quad (18)$$

This is essentially the Euler-Maclaurin summation formula. Since only simple calculus was used, this derivation is clearer than the operator derivation given earlier. The last integral, which is regarded as the remainder term, involves $B_{2n+1}(x)$ which has odd symmetry about $x = 1/2$. In general this causes cancellations making the remainder small. But making n very large does not always help since the maximum amplitude of $B_{2n+1}(x)$ in $(0,1)$ grows as n grows.

Combining and scaling intervals: Let the interval $[a, b]$ be split into n equal subintervals. Let

$$h = \frac{b-a}{n} \quad (19)$$

Then using a linear transformation of the variable we can show that

$$\int_a^b F(x)dx = T - \sum_{k=1}^{n} \frac{h^{2k}B_{2k}}{(2k)!}[F^{(2k-1)}(b) - F^{(2k-1)}(a)] - R \quad (20)$$

where,

$$T = h\left(\frac{1}{2}F(a) + F(a+h) + F(a+2h) + \ldots + F(a+(n-1)h) + \frac{1}{2}F(b)\right) \quad (21)$$

is the trapezoidal sum, and

$$R = \frac{h^{2n}}{(2n+1)!}\int_a^b B_{2n+1}\left(\frac{x-a}{h} \bmod 1\right)F^{(2n+1)}(x)dx \quad (22)$$

is the remainder term. It is worth noting the following points.

1. Only even powers of h appear in the difference between the trapezoidal sum and the integral. This is important in Romberg integration.

2. If the exact value of the integral is known, the Euler-Macluarin summation formula can be used for estimating a sum. This was its original use. It is widely used for summing slowly convergent series.