Bernoulli Numbers

Bernoulli numbers are named after the great Swiss mathematician Jacob Bernoulli(1654-1705) who used these numbers in the power-sum problem. The power-sum problem is to find a formula for the sum of the r-th powers of the first n natural numbers for positive integer exponents r.

$$\sigma_r(n) = 1^r + 2^r + \ldots + n^r \tag{1}$$

For small values of r expressions for $\sigma_r(n)$ are well known. For example

$$\sigma_1(n) = \tfrac{n(n+1)}{2} \tag{2}$$

$$\sigma_2(n) = \tfrac{n(n+1)(2n+1)}{6} \tag{3}$$

$$\sigma_3(n) = \left[\tfrac{n(n+1)}{2}\right]^2 \tag{4}$$

We will not follow Bernoulli's original method. We will use a shortcut involving the differentiation operator $\mathbf{D}$. To simplify the presentation we will consider the sum of the r-th powers till $n-1$.

$$S_r(n) = 1^r + 2^r + \ldots + (n-1)^r = \sum_{k=0}^{n-1} k^r \tag{5}$$

$S_r(n)$ satisfies the difference equation

$$S_r(n+1) - S_r(n) = n^r \tag{6}$$

with initial condition

$$S_r(0) = 0 \tag{7}$$

It is easy to derive an expression for $S_r(n)$ for the first few values of r.

$$S_1(n) = \tfrac{n(n-1)}{2} = \frac{n^2}{2} - \frac{n}{2} \tag{8}$$

$$S_2(n) = \tfrac{n(n-1)(2n-1)}{6} = \frac{n^3}{3} - \frac{n^2}{2} + \frac{n}{6} \tag{9}$$

$$S_3(n) = \tfrac{n^2(n-1)^2}{4} = \frac{n^4}{4} - \frac{n^3}{2} + \frac{n^2}{4} \tag{10}$$

$$S_4(n) = \tfrac{n(n-1)(2n-1)(3n^2-3n-1)}{30} = \frac{n^5}{5} - \frac{n^4}{2} + \frac{n^3}{3} - \frac{n}{30} \tag{11}$$

From this small list we observe that the polynomial $S_r(n)$ seems have the following interesting properties.

- The leading term of $S_r(n)$ is $\frac{n^{r+1}}{r+1}$. The next term is $-\frac{n^r}{2}$.
- $S_r(0) = S_r(1) = 0$
- $S_r(-n) = (-1)^{r+1} S_r(n+1)$
- $S_r(n)$ has factors n, $(n-1)$. When r is even, $(2n-1)$ is also a factor.

Operator-based Solution: In the past we have discussed how the Taylor series

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \ldots \tag{12}$$

may be written as

$$f(x+h) = e^{h\mathbf{D}} f(x) \tag{13}$$

where $\mathbf{D}$ is the differentiation operator. We write $S_r(n+1) - S_r(n) = n^r$ as

$$(e^{\mathbf{D}} - 1) S_r(n) = n^r \tag{14}$$

where the operator $\mathbf{D}$ means differentiation with respect to n. A formal solution is

$$S_r(n) = \frac{1}{e^{\mathbf{D}} - 1} n^r = \frac{\mathbf{D}}{e^{\mathbf{D}} - 1} \mathbf{D}^{-1} n^r = \frac{\mathbf{D}}{e^{\mathbf{D}} - 1} \left(\frac{n^{r+1}}{r+1} + C \right) \tag{15}$$

where C is a constant of integration to be determined from $S_r(0) = 0$. Note that the $\mathbf{D}^{-1}$ factor was separated so that $\frac{\mathbf{D}}{e^{\mathbf{D}}-1}$ only contains positive powers of $\mathbf{D}$. Now all that is needed is a power series expansion for $\frac{\mathbf{D}}{e^{\mathbf{D}}-1}$ in powers of $\mathbf{D}$.

Definition:

$$\frac{z}{e^z - 1} = \sum_{k=0}^{\infty} B_k \frac{z^k}{k!} \tag{16}$$

The numbers $B_k,\ k = 0, 1, 2, \ldots$ are known as **Bernoulli numbers**. Many problems in analysis can be solved using Bernoulli numbers. Since $z/(e^z - 1)$ has simple poles at $z = \pm 2\pi n i$, $n = 1, 2, \ldots$, the expansion here converges for $|z| < 2\pi$.

Properties: By letting $z \to 0$ in the definition we see that

$$B_0 = 1 \tag{17}$$

Next we see that

$$\frac{z}{2} + \frac{z}{e^z - 1} = \frac{z}{2}\frac{e^z + 1}{e^z - 1} = \frac{z}{2}\coth\frac{z}{2} \tag{18}$$

is an even function of z. So in its power series expansion about $z = 0$ the odd order coefficients are zero. So $B_1 + \frac{1}{2}$, B_3, B_5, B_7, ... are zero. This means that

$$B_1 = -\frac{1}{2} \tag{19}$$

$$B_{2k+1} = 0, \ \ k = 1, 2, 3, \ldots \tag{20}$$

A **recurrence formula** for the computation of the Bernoulli numbers will now be given.

$$\frac{z}{e^z - 1} e^z = z + \frac{z}{e^z - 1} \tag{21}$$

$$\Rightarrow \left(\sum_{k=0}^{\infty} B_k \frac{z^k}{k!}\right)\left(\sum_{m=0}^{\infty} \frac{z^m}{m!}\right) = z + \sum_{n=0}^{\infty} B_n \frac{z^n}{n!} \tag{22}$$

On the left hand side there is the product of two power series. The first is from the definition of the Bernoulli numbers, and the second is the power series for the exponential function. We recall the rule for multiplying two power series. If

$$\left(\sum_{k=0}^{\infty} a_k z^k\right)\left(\sum_{m=0}^{\infty} b_m z^m\right) = \left(\sum_{n=0}^{\infty} c_n z^n\right) \tag{23}$$

then

$$c_n = \sum_{k=0}^{n} a_k b_{n-k} \tag{24}$$

Thus applying this rule to equation (22) we get

$$\sum_{n=0}^{\infty}\left(\sum_{k=0}^{n} \frac{B_k}{k!(n-k)!}\right) z^n = z + \sum_{n=0}^{\infty} B_n \frac{z^n}{n!} \tag{25}$$

We compare coefficients of z^n on both sides for $n > 1$ to obtain

$$\frac{B_n}{n!} = \sum_{k=0}^{n} \frac{B_k}{k!(n-k)!} \tag{26}$$

(Since B_0 and B_1 are already known we only care about $n > 1$.)

$$\Rightarrow B_n = \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} B_k = \sum_{k=0}^{n} \binom{n}{k} B_k, \ \ n > 1 \tag{27}$$

This relation can be symbolically written as

$$B_n = (1 + B)_n, \quad n > 1 \tag{28}$$

where $(1 + B)_n$ is to be expanded just like a binomial expansion except that instead of taking superscripts to get powers such as B^k we take subscripts to get the various Bernoulli numbers B_k. Actually since the B_n term cancels from both sides, we get a relation involving Bernoulli numbers till B_{n-1}. So

$$B_0 + nB_1 + \frac{n(n-1)}{2} B_2 + \ldots + \binom{n}{n-2} B_{n-2} + nB_{n-1} + B_n = B_n, \quad n > 1 \tag{29}$$

actually gives

$$B_{n-1} = -\frac{1}{n}\left(B_0 + nB_1 + \frac{n(n-1)}{2}B_2 + \ldots + \binom{n}{n-2}B_{n-2}\right) = -\frac{1}{n}\sum_{k=0}^{n-2}\binom{n}{k}B_k, \quad n > 1 \tag{30}$$

In this formula nearly half the terms on the right hand side do not contribute anything since $B_3 = B_5 = B_7 = \ldots = 0$. We show the use of (30) to compute B_2 and B_4.

$$B_2 = -\frac{1}{3}(B_0 + 3B_1) = -\frac{1}{3}\left(1 + 3\frac{-1}{2}\right) = \frac{1}{6} \tag{31}$$

B_3 is known to be 0.

$$B_4 = -\frac{1}{5}(B_0 + 5B_1 + 10B_2 + 10B_3) = -\frac{1}{5}\left(1 + 5\frac{-1}{2} + 10\frac{1}{6} + 10 \times 0\right) = -\frac{1}{30} \tag{32}$$

Exercise: Using a suitable arbitrary precision arithmetic package write a program to compute B_k in fractional form. Compare your program output with the table given here.

n	B_n
2	1/6
4	−1/30
6	1/42
8	−1/30
10	5/66
12	−691/2730
14	7/6
16	−3617/510
18	43867/798
20	−174611/330
22	854513/138
24	−236364091/2730
26	8553103/6
28	−23749461029/870
30	8615841276005/14322
32	−7709321041217/510
34	2577687858367/6
36	−26315271553053477373/1919190
38	2929993913841559/6
40	−261082718496449122051/13530

What many consider to be the **first computer program in the world** was written to compute the Bernoulli numbers by Lady Ada Lovelace(1815-1852) for the Analytical Engine of Charles Babbage(1791-1871).

Exercise: Show that

$$S_r(n) = \frac{1}{r+1}\sum_{k=0}^{r}\binom{r+1}{k}B_k n^{r+1-k} \tag{33}$$

What is $S_{10}(n)$? Compute $S_{10}(1000)$.

Expansions of some functions: From (16) and the even function of z in (18) it is clear that

$$\frac{z}{2}\coth\frac{z}{2} = \sum_{k=0}^{\infty}\frac{B_{2k}}{(2k)!}z^{2k}, \quad |z| < 2\pi \tag{34}$$

Substituting $2z$ for z we get

$$z\coth z = \sum_{k=0}^{\infty}\frac{2^{2k}B_{2k}}{(2k)!}z^{2k}, \quad |z| < \pi \tag{35}$$

Substituting iz for z we get

$$z\cot z = \sum_{k=0}^{\infty}(-1)^k\frac{2^{2k}B_{2k}}{(2k)!}z^{2k}, \quad |z| < \pi \tag{36}$$

Since $\cot z$ has simple poles at $z = k\pi$ where k can be any integer,

$$\cot z = \sum_{k=-\infty}^{\infty} \frac{c_k}{z - k\pi} \tag{37}$$

where the constants c_k are determined as

$$c_k = \lim_{z \to k\pi} (z - k\pi) \cot z = \lim_{z \to k\pi} \frac{z - k\pi}{\sin z} \cos z = 1 \tag{38}$$

It should be noted that the sum (37) is understood to be the limit as N tends to infinity of the sum of terms from $k = -N$ to $k = N$. So

$$\cot z = \frac{1}{z} + \sum_{k=1}^{\infty} \left(\frac{1}{z - k\pi} + \frac{1}{z - k\pi} \right) = \frac{1}{z} + 2 \sum_{k=1}^{\infty} \frac{z}{z^2 - (k\pi)^2} \tag{39}$$

and

$$z \cot z = 1 + 2 \sum_{k=1}^{\infty} \frac{z^2}{z^2 - (k\pi)^2} = 1 - 2 \sum_{k=1}^{\infty} \frac{\left(\frac{z}{k\pi}\right)^2}{1 - \left(\frac{z}{k\pi}\right)^2} \tag{40}$$

This expansion is valid at all values of z except nonzero multiples of π. If we restrict z to the inside of the circle of radius π with centre at the origin, then $|z/(k\pi)| < 1$ on the right hand side. But

$$\frac{u}{1 - u} = u + u^2 + u^3 + \ldots = \sum_{n=1}^{\infty} u^n, \quad |u| < 1 \tag{41}$$

So

$$z \cot z = 1 - 2 \sum_{k=1}^{\infty} \sum_{n=1}^{\infty} \left(\frac{z^2}{k^2 \pi^2} \right)^n = 1 - 2 \sum_{k=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{k^{2n}} \frac{z^{2n}}{\pi^{2n}} = 1 - 2 \sum_{n=1}^{\infty} \left(\sum_{k=1}^{\infty} \frac{1}{k^{2n}} \right) \frac{z^{2n}}{\pi^{2n}}, \quad |z| < \pi \tag{42}$$

The sum of inverse powers of the natural numbers is the famous zeta function of Riemann. When the real part of the argument is greater than 1 the zeta function can be defined by

$$\zeta(s) = \frac{1}{1^s} + \frac{1}{2^s} + \frac{1}{3^s} + \ldots = \sum_{k=1}^{\infty} \frac{1}{k^s}, \quad (\Re(s) > 1) \tag{43}$$

Now

$$z \cot z = 1 - 2 \sum_{n=1}^{\infty} \frac{\zeta(2n)}{\pi^{2n}} z^{2n} \tag{44}$$

But by (36)

$$z \cot z = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n 2^{2n} B_{2n}}{(2n)!} z^{2n} \tag{45}$$

Comparing coefficients of z^{2n} for $n = 1, 2, \ldots$ in (45) and (44) we get

$$\zeta(2n) = \frac{(-1)^{n-1} 2^{2n-1} B_{2n}}{(2n)!} \pi^{2n} \tag{46}$$

In particular

$$\zeta(2) = \frac{\pi^2}{6} \tag{47}$$

$$\zeta(4) = \frac{\pi^4}{90} \tag{48}$$

$$\zeta(6) = \frac{\pi^6}{945} \tag{49}$$

$$\zeta(8) = \frac{\pi^8}{9450} \tag{50}$$

Since for any natural number n, $\zeta(2n)$ is positive, (46) shows that B_{2n} has the same sign as $(-1)^{n-1}$ for positive n. In other words successive even index Bernoulli numbers alternate in sign starting with B_2. (There is no change in sign from $B_0 = 1$ to $B_2 = 1/6$.)

Exercise: Find

$$S = \sum_{k=0}^{\infty} \frac{1}{(2k+1)^4} = \frac{1}{1^4} + \frac{1}{3^4} + \frac{1}{5^4} + \ldots$$

The Euler-Maclaurin Summation Formula (Operator Derivation)

This is a formula relating sums to integrals. In analysis integrals are frequently easier to find than similar sums and the Swiss mathematician L. Euler(1707-1783) used this formula first to estimate sums in terms of the integrals. In direct numerical work integrals must be approximated by sums and the Scottish mathematician C. Maclaurin(1698-1746) used this formula to estimate an integral in terms of a trapezoidal sum. The Euler-Maclaurin formula is important not only because of the high accuracy it provides in numerical work but also because of the asymptotic forms which originate from it. Stirling's approximation for the factorial can be derived using the Euler-Maclaurin summation formula. Let

$$F(x) = \int_c^x f(\xi)\,d\xi = \mathbf{D}^{-1} f(x) \tag{51}$$

so that

$$\mathbf{D}F(x) = f(x) \tag{52}$$

and

$$\mathbf{D}^m F(x) = F^{(m)}(x) = f^{(m-1)}(x) \tag{53}$$

Now

$$\begin{aligned}
\frac{h}{2}\left[f(x+h) + f(x)\right] &= \frac{h}{2}(e^{h\mathbf{D}} + 1) f(x) = \frac{h\mathbf{D}}{2}(e^{h\mathbf{D}} + 1)\mathbf{D}^{-1} f(x) = \frac{h\mathbf{D}}{2}(e^{h\mathbf{D}} + 1) F(x) \\
&= \frac{h\mathbf{D}}{2}\frac{e^{h\mathbf{D}} + 1}{e^{h\mathbf{D}} - 1}(e^{h\mathbf{D}} - 1) F(x) = \frac{h\mathbf{D}}{2}\frac{e^{h\mathbf{D}} + 1}{e^{h\mathbf{D}} - 1}(F(x+h) - F(x)) \\
&= \frac{h\mathbf{D}}{2}\coth\frac{h\mathbf{D}}{2}(F(x+h) - F(x)) = \left(1 + \sum_{k=1}^{\infty}\frac{B_{2k}}{(2k)!}(h\mathbf{D})^{2k}\right)(F(x+h) - F(x)) \\
&= F(x+h) - F(x) + \sum_{k=1}^{\infty}\frac{B_{2k}h^{2k}}{(2k)!}\left[F^{(2k)}(x+h) - F^{(2k)}(x)\right] \\
&= \int_c^{x+h} f(\xi)\;d\xi - \int_c^x f(\xi)\;d\xi + \sum_{k=1}^{\infty}\frac{B_{2k}h^{2k}}{(2k)!}\left[f^{(2k-1)}(x+h) - f^{(2k-1)}(x)\right] \\
&= \int_x^{x+h} f(\xi)\;d\xi + \sum_{k=1}^{\infty}\frac{B_{2k}h^{2k}}{(2k)!}\left[f^{(2k-1)}(x+h) - f^{(2k-1)}(x)\right] \qquad (54)
\end{aligned}$$

Because the sum on the right hand side involves differences of end point derivatives only, telescoping can be used to express any trapezoidal sum in the following way.

$$\begin{aligned}
&h\left[\frac{1}{2}f(x) + f(x+h) + \ldots + f(x+(n-1)h) + \frac{1}{2}f(x+nh)\right] \\
&= \int_x^{x+nh} f(\xi)\;d\xi + \sum_{k=1}^{\infty}\frac{B_{2k}h^{2k}}{(2k)!}\left[f^{(2k-1)}(x+nh) - f^{(2k-1)}(x)\right] \qquad (55)
\end{aligned}$$

This is the celebrated Euler-Maclaurin summation formula. It shows the following remarkable facts.

- (TRAPEZOIDAL SUM) = (INTEGRAL) + (CORRECTION)
- The correction depends on derivatives of odd order only at the end points.
- The correction involves **only even powers** of the step size h. This fact makes Romberg integration a great success.
- The sum on the right hand side is often *asymptotic* in nature.
- This formula uses the Bernoulli numbers.

The derivation just presented is not rigorous and gives no estimate of the error if one uses only a finite number terms in the correction. A rigorous derivation will be presented later.