Queen Mary
University of London

C50 Enumerative & Asymptotic Combinatorics

Notes 9 **Spring 2003**

We saw in Part 1 an asymptotic estimate for $n!$ which began by comparing $\log n! = \sum_{i=1}^{n} \log i$ to $\int_1^n \log x \,\mathrm{d}x$. Obviously the comparison is not exact, but the approximation can often be improved by the Euler–Maclaurin sum formula. This formula involves the somewhat mysterious Bernoulli numbers, which crop up in a wide variety of other situations too.

Bernoulli numbers

The Bernoulli numbers B_n can be defined by the recurrence relation

$$B_0 = 1, \quad \sum_{k=0}^{n} \binom{n+1}{k} B_k = 0 \text{ for } n \geq 1.$$

Note that we can write the recurrence as

$$\sum_{k=0}^{n+1} \binom{n+1}{k} B_k = B_{n+1},$$

since the term B_{n+1} cancels from this equation (which expresses B_n in terms of earlier terms).

Conway and Guy, in *The Book of Numbers*, have a typically elegant presentation of the Bernoulli numbers. They write this relation as

$$(B+1)^{n+1} = B^{n+1}$$

for $n \geq 1$, where B^k is to be interpreted as B_k *after* the left-hand expression has been evaluated using the Binomial Theorem.

Thus,

$$B_2 + 2B_1 + 1 = B_2, \quad \text{whence} \quad B_1 = -\frac{1}{2},$$

$$B_3 + 3B_2 + 3B_1 + 1 = B_3, \quad \text{whence} \quad B_2 = \frac{1}{6},$$

and so on. Note that, unlike most of the sequences we have considered before, the Bernoulli numbers are not integers.

Theorem 1 *The exponential generating function for the Bernoulli numbers is*

$$\sum_{n\geq 0} \frac{B_n x^n}{n!} = \frac{x}{\exp(x)-1}.$$

Proof Let $F(x)$ be the e.g.f., and consider $F(x)(\exp(x)-1)$. The coefficient of $x^{n+1}/(n+1)!$ is

$$(n+1)!\sum_{k=0}^{n}\left(\frac{B_k}{k!}\right)\left(\frac{1}{(n+1-k)!}\right) = \sum_{k=0}^{n}\binom{n+1}{k}B_k = 0$$

for $n \geq 1$. (Note that the sum runs from 0 to n rather than $n+1$ because we subtracted the constant term from the exponential.) The coefficient of x, however, is clearly 1. So the product is x.

Corollary 2 $B_n = 0$ *for all odd* $n > 1$.

Proof

$$F(x)+\frac{x}{2} = \frac{x}{2}\cdot\frac{\exp(x/2)+\exp(-x/2)}{\exp(x/2)-\exp(-x/2)} = \frac{x}{2}\coth\left(\frac{x}{2}\right)$$

which is an even function of x; so the coefficients of the odd powers of x are zero.

Corollary 3

$$B_n = \sum_{k=1}^{n}\frac{(-1)^k k! S(n,k)}{k+1}.$$

Proof Let $f(x) = \log(1+x)/x = \sum a_n x^n/n!$, where

$$a_n = \frac{(-1)^n n!}{(n+1)}.$$

By Proposition 9 of Notes 2, $f(\exp(x)-1) = x/(\exp(x)-1) = \sum B_n x^n/n!$, where

$$B_n = \sum_{k=1}^{n} S(n,k)a_k.$$

One application of the Bernoulli numbers is in *Faulhaber's formula* for the sum of the kth powers of the first n natural numbers. Everyone knows that

$$\begin{aligned}\sum_{i=1}^{n} i &= n(n+1)/2,\\ \sum_{i=1}^{n} i^2 &= n(n+1)(2n+1)/6,\\ \sum_{i=1}^{n} i^3 &= n^2(n+1)^2/4,\end{aligned}$$

but how does the sequence continue?

Theorem 4

$$\sum_{i=1}^{n} i^k = \frac{1}{k+1}\sum_{j=0}^{k}\binom{k+1}{j}B_j(n+1)^{k+1-j}.$$

So, for example,

$$\begin{aligned}\sum_{i=1}^{n} i^4 &= \frac{1}{5}\left((n+1)^5-\frac{5}{2}(n+1)^4+\frac{5}{3}(n+1)^3-\frac{1}{6}(n+1)\right)\\ &= n(n+1)(6n^3+9n^2+n-1)/30.\end{aligned}$$

Proof This argument is written out in the shorthand notation of Conway and Guy. Check that you can turn it into a more conventional proof!

We calculate

$$(n+1+B)^{k+1}-(n+B)^{k+1}=\sum_{j=1}^{k+1}\binom{k+1}{j}n^{k-j}((B+1)^j-B^j).$$

Now $(B+1)^j = B^j$ for all $j \geq 2$, so the only surviving term in this expression is

$$(k+1)n^k((B+1)^1-B^1)=(k+1)n^k.$$

Thus we have

$$\frac{1}{k+1}((n+1+B)^{k+1}-(n+B)^{k+1})=n^k,$$

from which by induction we obtain

$$\frac{1}{k+1}((n+1+B)^{k+1}-B^{k+1})=\sum_{i=1}^{n} i^k.$$

The left-hand side of this expression is

$$\frac{1}{k+1}\sum_{j=0}^{k}\binom{k+1}{j}B_j(n+1)^{k+1-j},$$

as required.

Warning Conway and Guy use a non-standard definition of the Bernoulli numbers, as a result of which they have $B_1 = 1/2$ rather than $-1/2$. As a result, their formulae look a bit different.

How large are the Bernoulli numbers? The generating function $x/(\exp(x)-1)$ has a removable singularity at the origin; apart from this, the nearest singularities are at $\pm 2\pi\mathrm{i}$, and so B_n is about $n!(2\pi)^{-n}$; in fact, it can be shown that

$$|B_n| = \frac{2\,n!\,\zeta(n)}{(2\pi)^n}$$

for n even, where $\zeta(n) = \sum_{k\geq 1} k^{-n}$. Of course, $B_n = 0$ if n is odd and $n > 1$.

Another curious formula for B_n is due to von Staudt and Clausen:

$$B_{2n} = N - \sum_{p-1|2n}\frac{1}{p}$$

for some integer N, where the sum is over the primes p for which $p-1$ divides $2n$.

Bernoulli polynomials

The *Bernoulli polynomials* $B_n(t)$ are defined by the formula

$$\frac{x\exp(tx)}{\exp(x)-1} = \sum_{n\geq 0}\frac{B_n(t)x^n}{n!}.$$

Proposition 5 *The Bernoulli polynomials satisfy the following conditions:*

(a) $B_n(0) = B_n(1) = B_n$ *for* $n \neq 1$, *and* $B_1(0) = -1/2$, $B_1(1) = 1/2$..

(b) $B_n(t+1) - B_n(t) = nt^{n-1}$.

(c) $B_n'(t) = nB_{n-1}(t)$.

(d) $B_n(t) = \sum_{k=0}^{n}\binom{n}{k}B_{n-k}t^k$

Proof All parts are easy exercises. Let $F(t) = x\exp(tx)/(\exp(x)-1)$.

(a) $F(0)$ is the e.g.f. for the regular Bernoulli numbers, and $F(1) = x + F(0)$.
(b) $F(t+1) - F(t) = x\exp(tx)$.
(c) $F'(t) = xF(t)$.
(d) $F(t) = F(0)\exp(xt)$: use the rule for multiplying e.g.f.s.

The first few Bernoulli polynomials are

$$B_0(t) = 1, \qquad B_1(t) = t - \tfrac{1}{2}, \qquad B_2(t) = t^2 - t + \tfrac{1}{6},$$
$$B_3(t) = t^3 - \tfrac{3}{2}t^2 + \tfrac{1}{2}t, \qquad B_4(t) = t^4 - 2t^3 + t^2 - \tfrac{1}{30}.$$

The Euler–Maclaurin sum formula

Faulhaber's formula gives us an exact value for the sum of the values of a polynomial over the first n natural numbers. The Euler–Maclaurin formula generalises this to arbitrary well-behaved functions; instead of an exact value, we must be content with error estimates, which in some cases enable us to show that we have an asymptotic series.

The Euler–Maclaurin sum formula connects the sum

$$\sum_{i=1}^{n} f(i)$$

with the series

$$\int_1^n f(t)\,\mathrm{d}t + \frac{1}{2}(f(1)+f(n)) + \sum \frac{B_{2i}}{(2i)!}\left(f^{(2i-1)}(n) - f^{(2i-1)}(1)\right),$$

where f is a "sufficiently nice" function.

Here is a precise formulation due to de Bruijn.

Theorem 6 *Let f be a real function with continuous $(2k)$th derivative. Let*

$$S_k = \int_1^n f(t)\,\mathrm{d}t + \frac{1}{2}(f(1)+f(n)) + \sum_{i=1}^{k} \frac{B_{2i}}{(2i)!}\left(f^{(2i-1)}(n) - f^{(2i-1)}(1)\right).$$

Then

$$\sum_{i=1}^{n} f(i) = S_k - R_k,$$

where the error term is

$$R_k = \int_1^n f^{(2k)}(t)\frac{B_{2k}(\{t\})}{(2k)!}\,\mathrm{d}t,$$

with $B_{2k}(t)$ the Bernoulli polynomial and $\{t\} = t - \lfloor t \rfloor$ the fractional part of t.

Proof First let g be any function with continuous $(2k)$th derivative on $[0,1]$. We claim that

$$\frac{1}{2}(g(0)+g(1)) - \int_0^1 g(t)\,\mathrm{d}t = \sum_{i=1}^{k} \frac{B_{2i}}{(2i)!}\left(g^{(2i-1)}(1) - g^{(2i-1)}(0)\right) - \int_0^1 g^{(2k)}(t)\frac{B_{2k}(t)}{(2k)!}\,\mathrm{d}t.$$

The proof is by induction: both the start of the induction (at $k = 1$) and the inductive step are done by integrating the last term by parts twice, using the fact that $B_n'(t) = nB_{n-1}(t)$ (see Proposition 5).

Now the result is obtained by applying this claim successively to the functions $g(x) = f(x+1)$, $g(x) = f(x+2)$, $\ldots$, $g(x) = f(x+n-1)$, and adding.

If f is a polynomial, then $f^{(2k)}(x) = 0$ for sufficiently large k, and the remainder term vanishes, giving Faulhaber's formula. For other applications, we must estimate the size of the remainder term.

There are various analytic conditions which guarantee a bound on the size of R_k, so that it can be shown that we have an asymptotic series for the sum. I will not give precise conditions here.

Example: Stirling's formula Let $f(x) = \log x$. Then $f^{(k)}(x) = \frac{(-1)^{k-1}(k-1)!}{x^k}$. We obtain the asymptotic series

$$c + n\log n - n + \frac{1}{2}\log n + \sum \frac{B_{2k}}{2k(2k-1)n^{2k-1}}$$

for

$$\sum_{i=1}^{n} \log i = \log n!\,.$$

The series begins $1/(12n) - 1/(360n^3) + 1/(1260n^5) + \cdots$. Exponentiating term-by-term (using the fact that, if $\log X = \log Y + o(n^{-k})$ then $X = Y(1+o(n^{-k}))$), we obtain

$$n! \sim \sqrt{2\pi}\,\frac{n^{n+1/2}}{\mathrm{e}^n}\left(1 + \frac{1}{12n} + \frac{1}{288n^2} + \cdots\right).$$

Note in passing that, for fixed n, this asymptotic series is divergent (see our earlier estimate for B_k).

Example: The harmonic series Applying Euler–Maclaurin to $f(x) = 1/x$, we get

$$\sum_{i=1}^{n} \frac{1}{i} \sim \log n + \gamma - \sum \frac{B_k}{kn^k},$$

where the sum begins $1/(2n) - 1/(12n^2) + 1/(120n^4) + \cdots$. Here γ is the *Euler–Mascheroni constant* (or *Euler's constant*), a somewhat mysterious constant with value approximately $0.5772157\ldots$. Again the series is divergent for fixed n.