Report 7

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Chapter 6
Euler-Machlaurin Summation

This chapter is about numericial analysis of the roots which uses the Euler-Maclaurin summation. Euler-Maclaurin summaion is a techique for the numberical evaluation of sums. It also used to compute $\zeta(s)$ for $s = 2, 3, \ldots, 15, 16$, and to compute $\Pi(s)$ for large s. Gram's[1] work was carried further by Backlund, he uses a method of computing for certain values of T, the number of roots in the range $0 \leq Im\ s \leq T$. This enabled him to show that Riemman hypothesis is true up to the level $T = 200$. About 10 years later Hutchinson verified up to the level $T = 300$.

1. Euler-Maclaurin summation

   First consider the problem of finding the numerical value of the sum S

$$S = \left(\frac{1}{10}\right)^2 + \left(\frac{1}{20}\right)^2 + \left(\frac{1}{30}\right)^2 + \cdots + \left(\frac{1}{100}\right)^2$$

   This sum is approximated to $\int_{10}^{100} x^{-2}dx$, specifically, the trapezoidal rule

$$\int_a^b f(x)dx \sim \sum_{i=1}^{n} \frac{f(x_i) + f(x_{i-1})}{2}(x_i - x_{i-1})$$

   where $(a = x_0 < x_1 < \cdots < x_n = b)$, in the case $x_0 = 10, x_1 = 11, \ldots, x_n = 100, f(x) = x^{-2}$
   This gives

$$\int_{10}^{100} \frac{dx}{x^2} \sim \frac{1}{2}\left[\left(\frac{1}{10}\right)^2 + \left(\frac{1}{11}\right)^2\right] \cdot 1 + \frac{1}{2}\left[\left(\frac{1}{11}\right)^2 + \left(\frac{1}{12}\right)^2\right] \cdot 1 + \cdots + \frac{1}{2}\left[\left(\frac{1}{99}\right)^2 + \left(\frac{1}{100}\right)^2\right] \cdot 1$$

   Hence

$$S \sim \int_{10}^{100} \frac{dx}{x^2} + \frac{1}{2}\left(\frac{1}{10}\right)^2 + \frac{1}{2}\left(\frac{1}{100}\right)^2 = -\frac{1}{x}|_0^{100} + 0.005 + 0.00005 = -0.9505$$

   Euler-Machaurin summation is a method of computing the error in this approximation. and in the more general sense

$$\sum_{n=M}^{N} f(n) \sim \int_M^N f(x)dx + \frac{1}{2}[f(M) + f(N)]$$

[1] Gram published a list of 15 roots on the line $Re\ s = \frac{1}{2}$. He computed the first 10 of these roots to about 6 d.p. and remaining 5 to about 1 place.

the desired formula is

$$\sum_{n=M}^{N} f(n) = \int_M^N f(x)dx + \frac{1}{2}[f(M) + f(N)] + \int_M^N (x - [x] - \frac{1}{2})f'(x)dx$$

Now back to the summation S, this formula shows that its value is 0.09505 plus

$$\int_{10}^{100} \frac{(x - [x] - \frac{1}{2})(-2)}{x^3} dx$$

the integrand in this integral is positive from 10 to 10.5 and negative from 10.5 to 11,etc.. Since x^{-3} decreases, the integral can be written as an alternating series of terms which decrease in absolute value. so

$$\int_{10}^{10.5} \frac{(x - [x] - \frac{1}{2})(-2)}{x^3} dx = \int_0^{1/2} \frac{1 - 2t}{(10 + t)^3} dt \le \int_0^{1/2} (1-2t)dt = 0.00025$$

Therefore S lies between 0.09505 and 0.09530, which gives it's value to 3 d.p.

The real substance of Euler-Maclaurin summation is repeated integration by parts o fthe last term in the desired formula i.e. $\int_M^N (x-[x]-\frac{1}{2})f'(x)dx$, in this way the last term can be evaluated numerically with great accuracy. However this integration by parts requires the use of Bernoulli polynomials. The nth Bernoulli polynomial i sby definition the unique polynomial of degree n with the proerty that

$$\int_x^{x+1} B_n(t)dt = x^n$$

differentiate it gives

$$B_n(x + 1) - B_n(x) = nx^{n-1},$$
$$\int_x^{x+1} \frac{1}{n} B'_n(t)dt = x^{n-1}$$

which shows that

$$B'_n(x) = nB_{n-1}(x)$$

These polynomials can be sued to interate the last term in desired formula for $\sum f(n)$ put in the form

$$\int_M^N \left(x-[x]-\frac{1}{2}\right)f'(x)dx = \sum_{n+M}^{N-1}\int_0^1\left(t-\frac{1}{2}\right)f'(n+t)dt = \sum_{n=M}^{N-1}\int_0^1 B_1(t)f'(n+t)dt$$

$$= \sum_{n=M}^{N-1}\left[\frac{B_2(t)}{2}f'(n+t)|_0^1 - \frac{1}{2}\int_0^1 B_2 f''(n+t)\right]$$

$$= -\frac{B_2(0)}{2}f'(M) + \frac{B_2(1)}{2}f'(M+1) - \frac{B_2(0)}{2}f'(M+1)$$

$$+ \frac{B_2(1)}{2}f'(M+2) - \frac{B_2(0)}{2}f'(M+2) + \cdots + \frac{B_2(1)}{2}f'(N)$$

$$-\frac{1}{2}\int_M^N B_2(x-[x])f''(x)dx.$$

Now let $\overline{B}_2(x)$ denote the periodic function $B_2(x-[x])$ the last term can be written as

$$\frac{B_2(0)}{2}f'(x)|_M^N - \frac{1}{2}\int_M^N \overline{B}_2(x)f''(x)dx$$

The second term in this formula can be integrated by parts by the exactly the same sequence of steps to put the last term of the desired formula in the form

$$\frac{B_2(0)}{2}f'(x)|_M^N - \frac{B_3(0)}{2\cdot 3}f''(x\_M^N) + \frac{1}{2\cdot 3}\int_M^N \overline{B}_3(x)f'''(x)dx$$

where $\overline{B}_3(x)$ denotes the periodic function $B_3(x-[x])$. Applying this formula to the evaluation of the error term in S gives

$$\frac{\frac{1}{6}}{2}\frac{-2}{x^3}|_{10}^{100} - 0 + \frac{1}{2\cdot 3}\int_{10}^{100}\overline{B}_3(x)f'''(x)dx$$

$$= \frac{1}{6}\left[\frac{1}{10^3} - \frac{1}{100^3}\right] + \frac{(-2)(-3)(-4)}{2\cdot 3}\int_{10}^{100}\frac{\overline{B}_3(x)dx}{x^5}$$

$$= \frac{999}{6\cdot 10^6} - 4\int_{10}^{100}\frac{\overline{B}_3(x)dx}{x^5}$$

By this formula,

$$S = 0.09505 + 1.665 * 10^{-4} - 4\int_{10}^{100}\frac{\overline{B}_3(x)dx}{x^5}$$

lies in the range

$$0.095215875 \le S \le 0.0952165$$

which gives S to six places.

To sum up the Euler-Maclaurin summation formula is,

$$\sum_M^N f(n) = \int_M^N f(x)dx + \frac{1}{2}[f(M)+f(N)] + \frac{B_2}{2}f'(x)|_M^N + \frac{B_4}{4!}f'''(x)|_M^N + \cdots + \frac{B_{2\nu}}{(2\nu)!}f^{2\nu-1}(x)|_M^N + R_{2\nu}$$

where B_n are Bernoulli numbers, where f(x) is any funcion which has $2\nu + 1$ continuous derivatives on [M,N]. and where $R_{2\nu}$ is given by either fot the formula

$$R_{2\nu} = \frac{-1}{(2\nu)!} \int_M^N \overline{B}_{2\nu}(x) f^{(2\nu)}(x) dx$$

or

$$R_{2\nu} = \frac{-1}{(2\nu+1)!} \int_M^N \overline{B}_{2\nu+1}(x) f^{(2\nu+1)}(x) dx$$

2. Evaluation of Π by Euler-Maclaurin summation. Stirling's series

To evaluate $\Pi(s)$, it is suffice to evaluate $log\Pi(s)$. No if s is a postive integer, say $s = N$, then $log\Pi(N) = \sum_1^N logn$, so by Euler-Maclaurin summation,

$$\int_1^N logxdx + \frac{1}{2}[log1 + logN] + \int_1^N \frac{\overline{B}_1(x)dx}{x}$$

The first term can be evaluated using $\int logxdx = xlogx - x$ the second term approaches a zero as $N \to \infty$, and the third term can be regarded as

$$\int_1^N \frac{\overline{B}_1(x)dx}{x} = \int_1^\infty \frac{\overline{B}_1(x)dx}{x} - \int_N^\infty \frac{\overline{B}_1(x)dx}{x}$$

So all these will give that

$$log\Pi(N) = \left(N + \frac{1}{2}\right) logN - N + A - \int_N^\infty \frac{\overline{B}_1(x)dx}{x}$$

where A is a constant

$$A = 1 + \int_1^\infty \frac{\overline{B}_1(x)dx}{x}$$

As it stands this formula cannot be valid for all real numbers N, since the derivative of its right hand side with respect to N is discontinuous at all integers. However if we rewritten in the form

$$log\Pi(s) = \left(s + \frac{1}{2}\right) logs - s + A - \int_0^\infty \frac{\overline{B}_1(t)dt}{t+s}$$

In this way, both side of the equation are well-behaved functions of s for all real numbers.
Now combine this formula with Lenendre relation $\Pi(2s) = \frac{1}{\pi^{1/2}} 2^{2s} \Pi(s) \Pi\left(s - \frac{1}{2}\right)$ to give the value of the constant A. Up to now rewrite the formula of $\Pi(s)$ as

$$\Pi(s) = s^{s+(1/2)} e^{-s} e^A r(s)$$

where $r(s) = exp[-\int_0^\infty \frac{\overline{B}_1(t)dt}{s+t}]$. Then $r(s) \to 1$ as $s \to \infty$ so now the Lengendre relation says

$$(2s)^{2s+(1/2)}e^{-2s}e^{A}r(2s)$$
$$= \pi^{-1/2}2^{2s}s^{s+(1/2)}e^{-s}e^{A}r(s)\left(s-\frac{1}{2}\right)^{s}e^{-s+(1/2)}e^{A}r\left(s-\frac{1}{2}\right)$$
$$2^{1/2}\left(1-\frac{1}{2s}\right)^{-s}e^{-1/2}\pi^{1/2}\frac{r(2s)}{r(s)r(s-\frac{1}{2})}=e^{A}$$

As $s \to \infty$ left side approaches $2^{1/2}e^{1/2}e^{-1/2}\pi^{1/2}\cdot 1 = (2\pi)^{1/2}$ so $A = \frac{1}{2}log2\pi$, therefore the formula for $log\Pi(s)$ becomes

$$log\Pi(s) = \left(s+\frac{1}{2}\right)logs - s + \frac{1}{2}log2\pi - \int_0^\infty \frac{\overline{B}_1(x)dx}{s+x}$$

Integrate the last term several times,

$$log\Pi(s) = \left(s+\frac{1}{2}\right)logs - s + \frac{1}{2}log2\pi + \frac{B_2}{2s} + \frac{B_4}{4\cdot 3\cdot s^3} + \cdots + \frac{B_{2\nu}}{2\nu(2\nu-1)s^{2\ni+1}} + R_{2\nu}$$

where

$$R_{2\nu} = -\int_0^\infty \frac{\overline{B}_{2\nu}(x)dx}{2\nu(s+x)^{2\nu}} = -\int_0^\infty \frac{\overline{B}_{2\nu+1}(x)dx}{(2\nu+1)(s+x)^{2\nu+1}}$$

This is known as Stirling's series.

To compute $log\Pi(s)$ with greater accuracy (better accuracy than Sterling series), then the formula

$$log\Pi(s) = log\Pi(s+N) - log(s+1) - log(s+2) - \cdots - log(s+N)$$

can be used. Given $\epsilon > 0$ there is an N such that Stirling's series can be used to compute $log(s+N)$ with an error of less than ϵ. this makes possible the evalutaion of $log\Pi(s)$ with any prescribed degree of accuracy.

So far we only consider s as an real number, in the numerical analysis of the roots ρ is the use of Stirling's series for complex values of s. Let the "slit plane" be the set of all complex number other than the negative reals and zero. Then all the terms of Stirling's series are defined throughout the slit plane and are analytic functions fo s. However the estimate of $|R_{2\nu}|$ cannot be used when s is not real, so some other method is required.[2]

Stieltjes proved that,

$$|R_{2\nu-2}| \leq \left(\frac{1}{cos\theta/2}\right)^{2\nu}\left|\frac{B_{2\nu}}{(2\nu)(2\nu-1)s^{2\nu-1}}\right|$$

where $s = re^{i\theta}$ and $-\pi \leq \theta \leq \pi$. This inequality says if $B_{2\nu}$ is the first term omitted in Stirling's series, then the magnitude of the error is at most $cos^{-2\nu}(\theta/2)$ times the magnitude of th efirst term omittted.

[2] $|R_{2\nu}|$ is needed if Stirling's series is to be used to compute $log\Pi(s)$ for complex s.

3. Evaluation of *zeta* by Euler-Maclaurin summation

Now apply Euler-Maclaurin summtion direct to $\zeta(s) = \sum_1^\infty n^{-s}$ $(Re\ s \geq 1)$ does not give a workable method of evaluation $\zeta(s)$, since the reminders are not at all small.

So need find a workable way, consider

$$\begin{aligned}
\sum_1^\infty n^{-s} - \sum_{n=1}^{N-1} n^{-s} &= \sum_{n=N}^\infty n^{-s} \\
\zeta(s) - \sum_{n=1}^{N-1} n^{-s} &= \int_N^\infty x^{-s}dx + \frac{1}{2}N^{-s} + \int_N^\infty \overline{B}_1(x)(-s)x^{-s-1}dx \\
\zeta(s) &= \sum_{n=1}^{N-1} n^{-s} + \frac{N^{1-s}}{s-1} + \frac{1}{2}N^{-s} + \frac{B_2}{2}sN^{-s-1} + \cdots \\
&+ \frac{B_{2\nu}}{(2\nu)!}s(s+1)\cdots(s+2\nu-2)N^{-s-2\nu+1} + R_{2\nu}
\end{aligned}$$

where

$$\begin{aligned}
R_{2\nu} &= -\frac{s(s+1)\cdots(s+2\nu-1)}{(2\nu)!}\int_N^\infty \overline{B}_{2\nu}(x)x^{-s-2\nu}dx \\
&= -\frac{s(s+1)\cdots(s+2\nu)}{(2\nu+1)!}\int_N^\infty \overline{B}_{2\nu+1}(x)x^{-s-2\nu-1}dx
\end{aligned}$$

The same method by which Stieltjes estimated the remainder in Stirling's series can be applied to estimate the remainder $R_{2\nu}$, it gives

$$|R_{2\nu-2}| \leq \left|\frac{s(s+1)\cdots(s+2\nu-1)B_{2\nu}N^{-\sigma-2\nu+1}}{(2\nu)!(\sigma+2\nu-1)}\right| = \left|\frac{s+2\nu-1}{\sigma+2\nu-1}\right| |B_{2\nu}\ term\ of\ \zeta(s)|$$

where $\sigma = Re\ s$. This interprets that if $B_{2\nu}$ is the first term omitted, then the magnitude of the remainder is the series $\zeta(s)$ is at most $|s+2\nu-1|(\sigma+2\nu-1)^{-1}$ times the magnitude of the first term omitted.

4. Techniques for locating roots on the line

The function $\xi(s) = \Pi(s/2)\pi^{-s/2}(s-1)\zeta(s)$, it real valued on the line $Re\ s = \frac{1}{2}$, so it can be shown to have zeros on the line by showing that it changes sign.

Consider the problem determining the sign of $\xi(\frac{1}{2}+it)$, it can be rewritten in the form

$$\begin{aligned}\xi\left(\frac{1}{2}+it\right) &= \frac{s}{2}\Pi\left(\frac{s}{2}-1\right)]pi^{-s/2}(s-1)\zeta(s)\\ &= e^{log\Pi[(s/2)-1]}\pi^{-s/2}\cdot\frac{s(s-1)}{2}\cdot\zeta(s)\\ &= \left[e^{Relog\Pi[(s/2)-1]}\pi^{-1/4}\cdot\frac{-t^2-\frac{1}{4}}{2}\right]\\ &\times\left[e^{i\ Imlog\Pi[(s/2)-1]}\pi^{-it/2}\zeta\left(\frac{1}{2}+it\right)\right]\end{aligned}$$

where $s=\frac{1}{2}+it$, so now the sing of $\xi(\frac{1}{2}+it)$ is oppositeto the sign of the factor in the second set of brackets. Let Z(t) denote the the second factor.

$$Z(t)=e^{i\vartheta(t)}\zeta(\frac{1}{2}+it)$$

where $\vartheta(t)=Imlog\Pi\left(\frac{it}{2}-\frac{3}{4}\right)-\frac{t}{2}log\pi$
Now $vartheta(t)$ can be simplified to

$$\vartheta(t)=\frac{t}{2}log\frac{t}{2\pi}-\frac{t}{2}-\frac{\pi}{8}+\frac{1}{48t}+\frac{7}{5760t^3}+\cdots$$

therefore

$$\vartheta(t)\sim\frac{t}{2}log\frac{t}{2\pi}-\frac{t}{2}-\frac{\pi}{8}+\frac{1}{48t}$$

and the error approximation is very slight, and it is (by Sterling's series) less than

$$\begin{aligned}\frac{1}{cos^6\frac{\theta}{2}}\cdot\left|\frac{1}{42\cdot6\cdot5\left(\frac{it}{2}+\frac{1}{4}\right)^5}\right| &\le \frac{1}{t^5}\frac{2^3}{42\cdot6\cdot\left(\frac{1}{2}\right)^5\left(1+\frac{1}{4t^2}{}^{5/2}\right)}\\ &\le \frac{1}{t^5}\cdot\frac{64}{63}\end{aligned}$$

and the errorsresultingfrom truncatingthe alternating series are less thanthe first term omittedwhich gives a total error of less than $\frac{1}{t^5}$
So the totalerrorinthe approximation of $\vartheta(t)$ is definitly less than

$$\frac{7}{5760t^3}+\frac{2}{t^5}$$

5. Techniques for computing the numbers of roots in a given range

The method for finding the root between the ranged was first developed by Gram, however his method rapidly becomes unworkableas the number of roots considered increases, so to extend the computations beyond 10 or 15 roots, a new method is required, such a method was found by Balcklund.

His method was based on Riemann's observation that if N(T) denotes the number of roots ρ in the range $0 < Ims < T$, then

$$N(T) = \frac{1}{2\pi} \int_{\partial R} \frac{\xi'(s)}{\xi(s)} ds$$

where R is a rectangle of the form $-\epsilon \leq Re\ s \leq 1+\epsilon, 0 \leq Im\ s \leq T$, and ∂R is in the anticlockwise direction, and it is assumed there are no roots ρ on the line $Im\ s = T$. By symmetry and the xi is real on the real axis, N(T) can be rewritten as

$$N(T) = \frac{1}{2\pi} \cdot 2Im \left[\int_C \frac{\xi'(s)}{\xi(s)} ds \right]$$

where C is the protion of ∂R from $1+\epsilon$ to $\frac{1}{2} + iT$

Backlund shows that there are no roots on C and he wrote

$$N(T) = \frac{1}{\pi}\vartheta + 1 + \frac{1}{\pi} \int_C \frac{\zeta'(s)}{\zeta(s)}$$

6. Backlund's estimate of N(T)

Riemann estimate of N(T) is the statement that the error in the approximation

$$N(T) \sim \frac{T}{2\pi} log \frac{T}{2\pi} - \frac{T}{2\pi}$$

is less than a constant times T^{-1}. However the formulas

$$N(T) = \frac{1}{\pi}\vartheta + 1 + \frac{1}{\pi} \int_C \frac{\zeta'(s)}{\zeta(s)}$$

and

$$\vartheta(t) = \frac{t}{2} log \frac{t}{2\pi} - \frac{t}{2} - \frac{\pi}{8} + \frac{1}{48t} + \frac{7}{5760t^3} + \cdots$$

of previous sections combine to give

$$N(T) - \left[\frac{T}{2\pi} log \frac{T}{2\pi} - \frac{T}{2\pi} \right] = \left[-\frac{1}{8} + \frac{1}{48\pi T} + \cdots \right] + 1 + \pi^{-1} Im \int_C \frac{\zeta'(s)}{\zeta(s)} ds$$

This shows that the magnitude of the absolute error is less than

$$1 + \pi^{-1} \left| Im \int_C \frac{\zeta'(s)}{\zeta(s)} ds \right|$$

by refining the estimate carefully, Backlund was able to obtain the specific estimate

$$\left| N(T) - \left(\frac{T}{2\pi} log \frac{T}{2\pi} - \frac{T}{2\pi} - \frac{7}{8} \right) \right| < 0.137 logT + 0.443 loglogT + 4.350$$

for all $T \geq 2$