less than $x^{-(1/2)+\epsilon}$. Since $\mathrm{Li}(x) \sim (x/\log x)$, this implies that the absolute error is eventually less than $x^{(1/2)+\epsilon}$, say for $x \geq c$. Then since

$$\begin{aligned}\theta(x) - x &= \int_c^x \log t \, d[\pi(t) - \mathrm{Li}(t)] + \text{const} \\ &= (\log x)[\pi(x) - \mathrm{Li}(x)] - \int_c^x \frac{\pi(t) - \mathrm{Li}(t)}{t} \, dt + \text{const},\end{aligned}$$

it follows that

$$|\theta(x) - x| \leq (\log x)x^{(1/2)+\epsilon} + \int_c^x t^{-(1/2)+\epsilon} \, dt + \text{const} \leq x^{(1/2)+2\epsilon}$$

for all sufficiently large x. Since

$$\theta(x) \leq \psi(x) \leq \theta(x) + \frac{\log x}{\log 2}\theta(x^{1/2}) \sim \theta(x) + \text{const}\, x^{1/2} \log x,$$

this implies immediately that $|\psi(x) - x| \leq x^{(1/2)+2\epsilon}$ for all sufficiently large x. But the formulas

$$-\frac{\zeta'(s)}{\zeta(s)} = \int_0^\infty x^{-s} \, d\psi(x) = s \int_1^\infty x^{-s-1}\psi(x) \, dx,$$

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

which hold for $\mathrm{Re}\, s > 1$, combine to give

$$-\frac{d}{ds} \log[(s-1)\zeta(s)] = 1 + s \int_1^\infty x^{-s-1}[\psi(x) - x] \, dx$$

for $\mathrm{Re}\, s > 1$. If $|\psi(x) - x| < x^{(1/2)+2\epsilon}$ for all large x, then the integral on the right converges throughout the halfplane $\mathrm{Re}\, s > \frac{1}{2} + 2\epsilon$. By analytic continuation the right side (which is analytic by differentiation under the integral sign) must be equal to the left side throughout the halfplane $\mathrm{Re}\, s > \frac{1}{2} + 2\epsilon$, which shows that $\zeta(s)$ could have no zeros in this halfplane. Thus if the relative error in $\pi(x) \sim \mathrm{Li}(x)$ is less than $x^{-(1/2)+\epsilon}$ for all $\epsilon > 0$, the Riemann hypothesis must be true.

5.6 A POSTSCRIPT TO DE LA VALLÉE POUSSIN'S PROOF

The Euler product formula for $\zeta(s)$ implies that for $\mathrm{Re}\, s > 1$

$$(1) \qquad \begin{aligned}\frac{1}{\zeta(s)} &= \prod_p \left(1 - \frac{1}{p^s}\right) = 1 - \frac{1}{2^s} - \frac{1}{3^s} - \frac{1}{5^s} + \frac{1}{6^s} - \cdots \\ &= \sum_{n=1}^\infty \frac{\mu(n)}{n^s},\end{aligned}$$

where, as in the Möbius inversion formula, $\mu(n)$ is 0 if n is divisible by a square, -1 if n is a product of an odd number of distinct prime factors, and

$+1$ if n is a product of an even number of distinct prime factors [$\mu(1) = 1$]. Since $\zeta(s)$ has a pole at $s = 1$, $[\zeta(s)]^{-1}$ has a zero at $s = 1$; so if (1) were valid for $s = 1$, it would say

(2) $0 = 1 - \frac{1}{2} - \frac{1}{3} - \frac{1}{5} + \frac{1}{6} - \frac{1}{7} + \frac{1}{10} - \frac{1}{11} - \frac{1}{13} + \frac{1}{14} + \frac{1}{15} - \cdots.$

This equation was stated by Euler [E5], but Euler quite often dealt with divergent series and his statement of this equation should not necessarily be understood to imply *convergence* of the series on the right but only *summability*. At any rate Euler did not give any proof that the series (2) was convergent, and the first proof of this fact was given by von Mangoldt [M2] in 1897. Von Mangoldt's proof is rather difficult and a much simpler proof of the formula (2), together with an estimate of the *rate* of convergence, was given by de la Vallée Poussin in 1899 in connection with his proof of the improved error estimate $\exp[-(c \log x)^{1/2}]$ in the prime number theorem.

Specifically, de la Vallée Poussin proved that there is a constant K such that

(3)
$$\left| \sum_{n<x} \frac{\mu(n)}{n} \right| < \frac{K}{\log x}$$

for all sufficiently large x. As $x \longrightarrow \infty$ this of course implies (2). De la Vallée Poussin's proof is based on two observations concerning the function $P(x)$ defined by

$$P(x) = \int_0^x t^{-1}\, d\psi(t) = \sum_{n<x} \frac{\Lambda(n)}{n},$$

namely, the observation that $P(x)$ is related to the series (2) by the formula

(4)
$$\sum_{n<x} \frac{\mu(n)}{n}\left[P\left(\frac{x}{n}\right) + \log n\right] \equiv 0$$

and the observation that an estimate of $P(x)$ can be derived from the estimate of $\psi(x)$ obtained in Section 5.3.

Consider first the proof of (4). The essence of this identity is the identity

$$\frac{d}{ds}\left[\frac{1}{\zeta(s)}\right] = -\left[\frac{\zeta'(s)}{\zeta(s)}\right]\left[\frac{1}{\zeta(s)}\right]$$

which, since $-\zeta'(s)/\zeta(s) = \sum \Lambda(n)n^{-s}$ and $[\zeta(s)]^{-1} = \sum \mu(n)n^{-s}$ for $\operatorname{Re} s > 1$, gives

(5)
$$\sum_{n=1}^{\infty} \frac{-\mu(n)\log n}{n^s} = \left[\sum_{j=1}^{\infty} \frac{\Lambda(j)}{j^s}\right]\left[\sum_{k=1}^{\infty} \frac{\mu(k)}{k^s}\right]$$
$$= \sum_{n=1}^{\infty} \frac{1}{n^s}\left[\sum_{jk=n} \Lambda(j)\mu(k)\right]$$

for $\operatorname{Re} s > 1$. It is natural to suppose that since these series have the same sum for all s they must be identical, and hence for all x

$$\sum_{n<x} \frac{-\mu(n) \log n}{n^s} = \sum_{n<x} \frac{1}{n^s}\Big[\sum_{jk=n} \Lambda(j)\mu(k)\Big] \tag{6}$$

which for $s = 1$ gives

$$-\sum_{n<x} \frac{\mu(n) \log n}{n} = \sum_{n<x} \sum_{jk=n} \frac{\Lambda(j)}{j} \cdot \frac{\mu(k)}{k}. \tag{7}$$

Now for every fixed $k \le n < x$ the sum on the left is over all integers j such that $jk < x$, that is, it is over all integers $j < x/k$, hence

$$-\sum_{n<x} \frac{\mu(n) \log n}{n} = \sum_{k<x} \frac{\mu(k)}{k} P\Big(\frac{x}{k}\Big)$$

from which (4) follows. The one step of the argument which requires further justification is the truncation (6) of the series (5). This is essentially a question of recovering the coefficients of a series $\sum A_n n^{-s}$ from a knowledge of its sum, which can be done by a technique similar to that used in Section 3.2 to recover $\Lambda(n)$ from $-\zeta'(s)/\zeta(s) = \sum \Lambda(n)n^{-s}$. Specifically, one can go directly from (5) to the desired equation (7) by using the identity

$$\begin{aligned} \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty}\Big[\sum_{n=1}^{\infty} \frac{A_n}{n^s}\Big]\frac{x^s\,ds}{s-1} &= x \cdot \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty}\Big[\sum_{n=1}^{\infty} \frac{A_n}{n}\Big(\frac{x}{n}\Big)^{s-1}\Big]\frac{ds}{s-1} \\ &= x \cdot \frac{1}{2\pi i}\int_{a-1-i\infty}^{a-1+i\infty}\Big[\sum_{n=1}^{\infty} \frac{A_n}{n}\Big(\frac{x}{n}\Big)^{t}\Big]\frac{dt}{t} \\ &= x \cdot \sum_{n<x} \frac{A_n}{n}, \end{aligned}$$

where the termwise integration in the last step is justified, by the same argument as before, whenever the A_n are such that $\sum (|A_n|/n)n^{-(a-1)} < \infty$, which is certainly the case for both series in (5) for large a. This completes the proof of (4).

Consider now the estimation of $P(x)$. The desired estimate is easily found heuristically by using

$$d\psi(x) = (1 - \sum x^{\rho-1} - \sum x^{-2n-1})\,dx$$

to find

$$dP(x) = x^{-1}\,d\psi(x) = (x^{-1} - \sum x^{\rho-2} - \sum x^{-2n-2})\,dx,$$

$$P(x) = \log x - \sum \frac{x^{\rho-1}}{\rho-1} + \sum \frac{x^{-2n-1}}{2n+1} + \text{const},$$

which indicates that $P(x) \sim \log x + \text{const}$ with an error which goes to zero faster than

$$\begin{aligned} \Big|\sum \frac{x^{\rho-1}}{\rho-1}\Big| &\le \Big|\sum \frac{x^{\rho-1}}{\rho}\Big| + \Big|\sum \frac{x^{\rho-1}}{\rho(\rho-1)}\Big| \\ &\le \exp[-(c \log x)^{1/2}] + \exp[-(c \log x)^{1/2}]. \end{aligned}$$

In order to prove this it suffices to write

$$\begin{aligned}
P(x) &= \int_0^x t^{-1}\,d\psi(t) = t^{-1}\psi(t)\Big|_0^x + \int_0^x t^{-2}\psi(t)\,dt \\
&= \frac{\psi(x)}{x} + \int_1^x t^{-2}\psi(t)\,dt \\
&= \frac{\psi(x)-x}{x} + \int_1^x t^{-1}\,dt + \int_1^x t^{-1}\frac{\psi(t)-t}{t}\,dt + 1 \\
&= \log x + \frac{\psi(x)-x}{x} + \int_1^x t^{-1}\frac{\psi(t)-t}{t}\,dt + 1.
\end{aligned}$$

The integral in the last expression converges as $x \longrightarrow \infty$ because if x increases to x', it increases for large x by less than

$$\begin{aligned}
\int_x^{x'} t^{-1}\exp[-(c\log t)^{1/2}]\,dt &= \frac{1}{c}\int_{c\log x}^{c\log x'} \exp(-u^{1/2})\,du \\
&= \frac{2}{c}\int_{(c\log x)^{1/2}}^{(c\log x')^{1/2}} e^{-v}v\,dv = \frac{2}{c}(-e^{-v}v - e^{-v})\Big|_{(c\log x)^{1/2}}^{(c\log x')^{1/2}} \\
&\leq \frac{2}{c}(c\log x)^{1/2}\exp[-(c\log x)^{1/2}] + \frac{2}{c}\exp[-(c\log x)^{1/2}].
\end{aligned}$$

Thus the above formula can be rewritten

$$P(x) = \log x + 1 + \int_1^\infty \frac{\psi(t)-t}{t^2}\,dt + \frac{\psi(x)-x}{x} - \int_x^\infty \frac{\psi(t)-t}{t^2}\,dt,$$

$$P(x) = \log x + C + \eta(x), \tag{8}$$

where C is the constant† $1 + \int_1^\infty t^{-2}[\psi(t) - t]\,dt$ and where the error $\eta(x)$ is less than

$$\left(1 + \frac{2}{c}\right)\exp[-(c\log x)^{1/2}] + \frac{2}{c}(c\log x)^{1/2}\exp[-(c\log x)^{1/2}]$$

for all x large enough that $[\psi(t) - t]/t \leq \exp[-(c\log t)^{1/2}]$ for $t \geq x$. Thus it is possible to choose $K' > 0$, $c > 0$ such that the error $\eta(x)$ is less than

†The constant c is in fact the negative of Euler's constant (see Section 3.8). To derive this fact, note first that C is $1 + \lim_{s\to 1}\int_1^\infty t^{-1-s}[\psi(t) - t]\,dt$ and then integrate by parts to find that it is the limit as $s \longrightarrow 1$ of $-s^{-1}\{[\zeta'(s)/\zeta(s)] + 1 - s + (s-1)^{-1}\}$ which is the limit as $s \longrightarrow 1$ of $-(d/ds)\log[(s-1)\zeta(s)]$. But the functional equation gives $(s-1)\zeta(s) = -\Pi(1-s)(2\pi)^{s-1}\zeta(1-s)2\sin(\pi s/2)$. Using the fact that the logarithmic derivative of ζ at 0 is $\log 2\pi$ while that of Π is $-\gamma$ (see Section 3.8), the result $C = -\gamma$ then follows. Since the left side of formula (2) of Section 4.1 is $P(x) - x^{-1}\psi(x) = \log x + C - 1 + \cdots$, this implies that the constant on the right is $-\gamma - 1$. The same fact can also be derived by setting $v = 0$ in the formula of the note of Section 4.3 and letting $u \longrightarrow 1$. Yet another proof that $C = \gamma$ is given in Section 12.10.

$K' \exp[-(c \log x)^{1/2}]$ for all $x \geq 0$. Then (4) and (8) combine to give

$$\sum_{n<x} \frac{\mu(n)}{n}\left[\log\left(\frac{x}{n}\right) + C - \eta\left(\frac{x}{n}\right) + \log n\right] \equiv 0,$$

$$(\log x + C) \sum_{n<x} \frac{\mu(n)}{n} \equiv \sum_{n<x} \frac{\mu(n)}{n}\eta\left(\frac{x}{n}\right),$$

$$\left|\sum_{n<x} \frac{\mu(n)}{n}\right| \leq \frac{\sum_{n<x} (1/n)K' \exp[-(c \log (x/n))^{1/2}]}{\log x + C},$$

and the desired inequality (3) will follow if it can be shown that

$$\sum_{n<x} \frac{1}{n} \exp\left[-\left(c \log \frac{x}{n}\right)^{1/2}\right]$$

remains bounded as $x \longrightarrow \infty$. Now the logarithmic derivative of the summand with respect to n (considered for the moment as a continuous variable) is

$$-\frac{1}{n} - \frac{1}{2}\left(c \log \frac{x}{n}\right)^{-1/2} \frac{cn}{x} \cdot \left(-\frac{x}{n^2}\right) = \frac{1}{n}\left[-1 + \frac{c}{2}\left(c \log \frac{x}{n}\right)^{-1/2}\right]$$

which is negative until

$$c/2 = [c \log (x/n)]^{1/2}, \qquad \log (x/n) = c/4, \qquad n = xe^{-c/4},$$

after which it is positive. Let N be the last integer before the sign change. Then

$$\begin{aligned}
&\sum_{n<x} \frac{1}{n} \exp\left[-\left(c \log \frac{x}{n}\right)^{1/2}\right] \\
&\quad\leq \exp[-(c \log x)^{1/2}] + \sum_{n=2}^{N} \frac{1}{n} \exp\left[-\left(c \log \frac{x}{n}\right)^{1/2}\right] \\
&\quad\quad + \sum_{N+1 \leq n < x-1} \frac{1}{n} \exp\left[-\left(c \log \frac{x}{n}\right)^{1/2}\right] \\
&\quad\quad + \frac{1}{x} \exp\left[-\left(c \log \frac{x}{x}\right)^{1/2}\right] \\
&\quad\leq 1 + \int_1^N \frac{1}{t} \exp\left[-\left(c \log \frac{x}{t}\right)^{1/2}\right] dt \\
&\quad\quad + \int_{N+1}^x \frac{1}{t} \exp\left[-\left(c \log \frac{x}{t}\right)^{1/2}\right] dt + \frac{1}{x} \\
&\quad\leq 1 + \int_1^x \frac{1}{t} \exp\left[-\left(c \log \frac{x}{t}\right)^{1/2}\right] dt + \frac{1}{x}
\end{aligned}$$

and it suffices to show that this integral remains bounded as $x \longrightarrow \infty$. But $u = x/t$ gives

$$\int_1^x \frac{1}{t} \exp\left[-\left(c \log \frac{x}{t}\right)^{1/2}\right] dt = \int_1^x \frac{1}{u} \exp[-(c \log u)^{1/2}]\, du$$

and it was shown above that this integral converges as $x \longrightarrow \infty$, so the proof of (3), and hence of (2), is complete.

Chapter 6

Numerical Analysis of the Roots by Euler–Maclaurin Summation

6.1 INTRODUCTION

The first substantial numerical information on the roots ρ was given by Gram [G5], who in 1903 published a list of 15 roots on the line $\operatorname{Re} s = \frac{1}{2}$. Gram computed the first 10 of these roots to about 6 decimal places and the remaining 5 to about 1 place. Specifically, the values he gave were $\rho = \frac{1}{2} + i\alpha$, where

$$\begin{aligned}
\alpha_1 &= 14.134\,725, & \alpha_6 &= 37.586\,176, & \alpha_{11} &= 52.8,\\
\alpha_2 &= 21.022\,040, & \alpha_7 &= 40.918\,720, & \alpha_{12} &= 56.4,\\
\alpha_3 &= 25.010\,856, & \alpha_8 &= 43.327\,073, & \alpha_{13} &= 59.4,\\
\alpha_4 &= 30.424\,878, & \alpha_9 &= 48.005\,150, & \alpha_{14} &= 61.0,\\
\alpha_5 &= 32.935\,057, & \alpha_{10} &= 49.773\,832, & \alpha_{15} &= 65.0.
\end{aligned}$$

Subsequent calculations have confirmed that these values are correct except, as Gram stated, for slight errors in the last place given. (For the correct values to 6 places see Haselgrove's tables [H8].) Gram was also able to prove that this list includes *all* of the roots ρ in the range $0 \le \operatorname{Im} s \le 50$ and thus to prove that the Riemann hypothesis is true in this range.

The basis of Gram's calculations was the straightforward method of Euler–Maclaurin summation to evaluate both the function ζ and the factorial function Π, and consequently to evaluate $\xi(s) = \Pi(\frac{1}{2}s)\pi^{-s/2}(s-1)\zeta(s)$. It is interesting from the point of view of the psychology of mathematical discovery to note that Gram had initially attempted more original and more complicated techniques but had met with very limited success. It was several years before he tried using the classical method of Euler–Maclaurin summation, and when he did he was surprised at the ease with which he was able to compute the numbers he had been searching for for so long.

Euler–Maclaurin summation is a technique for the numerical evaluation of sums which was developed in the early part of the eighteenth century. The original impetus came from Bernoulli's success in generalizing $\sum_{n=1}^{N} n = N(N+1)/2$ to find an analogous formula for $\sum_{n=1}^{N} n^k$ which involved the "Bernoulli numbers." Forms of the technique were used by Stirling and De Moivre as early as 1730, but the definitive statement of the method together with a proof of sorts did not come until around 1740 when it was published by Euler and, independently (see Cantor [C1]), by Maclaurin. Euler in his well-known calculus book [E6] included examples of the use of Euler–Maclaurin summation to compute $\zeta(s)$ for $s = 2, 3, \ldots, 15, 16$ and to compute $\Pi(s)$ for large s (Stirling's series), so Gram's computations are direct descendants of Euler's.

Gram's work was carried farther by Backlund [B3, B4] around 1912–1915. Backlund's major contribution was a method of computing, for certain values of T, the number of roots in the range $0 \leq \operatorname{Im} s \leq T$. This method enabled him to show that the Riemann hypothesis was true up to the level $T = 200$, that is, to prove that all of the roots in the range $0 \leq \operatorname{Im} s \leq 200$ lie on the line $\operatorname{Re} s = \frac{1}{2}$. It also enabled him to prove that Riemann's estimate [see (d) of Section 1.19] of the number of roots in $0 \leq \operatorname{Im} s \leq T$ for large T was correct, a fact which von Mangoldt had already proved in 1905 by a method which was more complicated. Backlund's proof of this fact is included in this chapter, even though it does not contribute to the numerical analysis of the roots, because it is a natural outgrowth of techniques which Backlund developed for the numerical analysis of the roots.

Some ten years later the Riemann hypothesis was verified up to the level $T = 300$ by Hutchinson [H11], who contributed some improvements of Gram's and Backlund's methods. As far as the distribution of the roots on the line $\operatorname{Re} s = \frac{1}{2}$ is concerned, Hutchinson showed that it is usually true in the range $0 \leq \operatorname{Im} s \leq 300$ that there is exactly one root between two consecutive Gram points (see Section 6.5)—in other words the set of roots and the set of Gram points usually separate each other—but that there are two slight exceptions to this rule in this range, the first near $\operatorname{Im} s = 282.5$ and the second near $\operatorname{Im} s = 295.5$.

Broadly speaking, the computations of Gram, Backlund, and Hutchinson contributed substantially to the plausibility of the Riemann hypothesis, but they gave no insight into the question of why it might be true or into the question of why Riemann might have been led to make such a hypothesis.

6.2 EULER–MACLAURIN SUMMATION

Consider the problem of finding the numerical value of the sum S defined by

$$S = \left(\frac{1}{10}\right)^2 + \left(\frac{1}{11}\right)^2 + \left(\frac{1}{12}\right)^2 + \cdots + \left(\frac{1}{100}\right)^2. \tag{1}$$

As a first approximation to S one might note that if half the first term and half the last term are omitted from S, then the sum which remains is an approximation to $\int_{10}^{100} x^{-2}\,dx$; specifically, the trapezoidal rule

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

$$(a = x_0 < x_1 < \cdots < x_n = b)$$

in the case $x_0 = 10$, $x_1 = 11, \ldots, x_n = 100$, $f(x) = x^{-2}$ 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

$$S \sim \int_{10}^{100} \frac{dx}{x^2} + \frac{1}{2}\left(\frac{1}{10}\right)^2 + \frac{1}{2}\left(\frac{1}{100}\right)^2 = -\frac{1}{x}\Big|_{10}^{100} + 0.005 + 0.00005 = 0.09505.$$

Euler–Maclaurin summation is a method of computing the error in this approximation and in the analogous approximation

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

for other sums.

The first step is to develop a closed formula for the error. Let $[x]$ denote, as usual, the largest integer less than or equal to x. Then the function $[x]$ is a step function which has jumps of one at integers, so the Stieltjes measure $d([x])$ assigns the weight one to integers and is zero elsewhere. Hence

$$\int_M^N f(x)\,d([x]) = \tfrac{1}{2}f(M) + f(M+1) + f(M+2) + \cdots + f(N-1) + \tfrac{1}{2}f(N),$$

where the usual convention of counting half the weight at an end point is followed. Thus to make the approximation (2) correct, the right side should be increased by

$$-\int_M^N f(x)\,dx + \int_M^N f(x)\,d([x]) = \int_M^N f(x)\,d([x] - x).$$

It is more natural to describe the measure $d([x] - x)$ as $d([x] - x + \frac{1}{2})$ because the function $[x] - x + \frac{1}{2}$ is positive half the time and negative half the time, and because it is zero when x is an integer (by the usual convention that at discontinuities the value is the average of the left-hand limit and the right-hand limit). Integration by parts then expresses the error in the form

$$\begin{aligned}\int_M^N f(x)\,d([x] - x + \tfrac{1}{2}) &= -\int_M^N ([x] - x + \tfrac{1}{2})\,df(x)\\ &= \int_M^N (x - [x] - \tfrac{1}{2})f'(x)\,dx.\end{aligned}$$

Having arrived at this formula by sketchy arguments based on Stieltjes integration, one can easily justify it using ordinary Riemann integration to find

$$\begin{aligned}\int_M^N (x - [x] - \tfrac{1}{2})f'(x)\,dx &= \sum_{n=M}^{N-1} \int_n^{n+1} (x - [x] - \tfrac{1}{2})f'(x)\,dx\\ &= \sum_{n=M}^{N-1} \int_0^1 (t - \tfrac{1}{2})f'(n + t)\,dt\\ &= \sum_{n=M}^{N-1} \left[(t - \tfrac{1}{2})f(n + t)\Big|_0^1 - \int_0^1 f(n + t)\,dt\right]\\ &= \sum_{n=M}^{N-1} [\tfrac{1}{2}f(n + 1) + \tfrac{1}{2}f(n)] - \sum_{n=M}^{N-1} \int_0^1 f(n + t)\,dt\\ &= \tfrac{1}{2}f(M) + f(M + 1) + f(M + 2) + \cdots\\ &\quad + f(N - 1) + \tfrac{1}{2}f(N) - \int_M^N f(x)\,dx\end{aligned}$$

which proves the desired formula

$$\sum_{n=M}^{N} f(n) = \int_M^N f(x)\,dx + \tfrac{1}{2}[f(M) + f(N)] + \int_M^N (x - [x] - \tfrac{1}{2})f'(x)\,dx \tag{3}$$

for continuously differentiable functions f on $[M, N]$.

In the case of the sum S in (1) this formula shows that its value is 0.09505 plus

$$\int_{10}^{100} \frac{(x - [x] - \frac{1}{2})(-2)}{x^3}\,dx. \tag{4}$$

The integrand in this integral is positive from 10 to $10\frac{1}{2}$, negative from $10\frac{1}{2}$ to 11, positive from 11 to $11\frac{1}{2}$, etc. Since x^{-3} decreases, the integral can thus be written as an alternating series of terms which decrease in absolute value, so its value is positive but less than

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

Thus S lies between 0.09505 and 0.09530, which gives its value to three places.

This much is quite elementary. The real substance of Euler–Maclaurin summation is *repeated integration by parts of the last term of* (3) which puts this term in a form that can in many cases be evaluated numerically with great accuracy. This integration by parts requires the use of *Bernoulli polynomials.* The nth Bernoulli polynomial is by definition the unique polynomial of degree n with the property that

$$\int_x^{x+1} B_n(t)\,dt = x^n. \tag{5}$$

Thus, for example, $B_3(x) = ax^3 + bx^2 + cx + d$ is determined by the equation

$$\begin{aligned} x^3 &= \int_x^{x+1} (at^3 + bt^2 + ct + d)\,dt \\ &= a\frac{(x+1)^4 - x^4}{4} + b\frac{(x+1)^3 - x^3}{3} + c\frac{(x+1)^2 - x^2}{2} \\ &\quad + d\frac{x + 1 - x}{1} \\ &= ax^3 + \left(\frac{3}{2}a + b\right)x^2 + (a + b + c)x \\ &\quad + \left(\frac{a}{4} + \frac{b}{3} + \frac{c}{2} + \frac{d}{1}\right) \end{aligned}$$

from which one finds successively $a = 1$, $b = -3/2$, $c = 1/2$, $d = 0$. It is easy to see that this process always yields a polynomial $B_n(x)$ satisfying (5) and, since a polynomial $p(x)$ which satisfies $\int_x^{x+1} p(t)\,dt \equiv 0$ must be identically zero, this suffices to prove that condition (5) defines a unique polynomial $B_n(x)$. Differentiation of (5) gives

$$B_n(x + 1) - B_n(x) = nx^{n-1}, \tag{6}$$
$$\int_x^{x+1} \frac{1}{n} B_n'(t)\,dt = x^{n-1},$$

which shows that $B_n'(x)/n$ satisfies the definition of $B_{n-1}(x)$ and hence that

$$B_n'(x) = nB_{n-1}(x). \tag{7}$$

Thus, starting with $B_3(x)$, which was computed above, one has immediately

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

These polynomials can be used to integrate the last term of (3) by parts to put it in the form

$$\begin{aligned}
&\int_M^N \left(x - [x] - \frac{1}{2}\right) f'(x)\,dx \\
&= \sum_{n=M}^{N-1} \int_0^1 \left(t - \frac{1}{2}\right) f'(n+t)\,dt = \sum_{n=M}^{N-1} \int_0^1 B_1(t) f'(n+t)\,dt \\
&= \sum_{n=M}^{N-1} \left[\frac{B_2(t)}{2} f'(n+t)\Big|_0^1 - \frac{1}{2}\int_0^1 B_2(t) f''(n+t)\,dt\right] \\
&= -\frac{B_2(0)}{2} f'(M) + \frac{B_2(1)}{2} f'(M+1) - \frac{B_2(0)}{2} f'(M+1) \\
&\quad + \frac{B_2(1)}{2} f'(M+2) - \frac{B_2(0)}{2} f'(M+2) + \cdots + \frac{B_2(1)}{2} f'(N) \\
&\quad - \frac{1}{2}\int_M^N B_2(x - [x]) f''(x)\,dx.
\end{aligned}$$

The long sum telescopes because (6) with $n = 2$, $x = 0$ gives $B_2(1) = B_2(0)$. Thus if $\bar{B}_2(x)$ is used to denote the periodic function $B_2(x - [x])$, the last term of (3) can be written in the form

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

The second term in this formula can be integrated by parts by exactly the same sequence of steps to put the last term of (3) in the form

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

where, of course, $\bar{B}_3(x)$ denotes the periodic function $B_3(x - [x])$.

Applying this formula to the evaluation of the integral (4) gives

$$\begin{aligned}
&\frac{\frac{1}{6}}{2}\,\frac{-2}{x^3}\Big|_{10}^{100} - 0 + \frac{1}{2\cdot 3}\int_{10}^{100} \bar{B}_3(x) f'''(x)\,dx \\
&= \frac{1}{6}\left[\frac{1}{10^3} - \frac{1}{100^3}\right] + \frac{(-2)(-3)(-4)}{2\cdot 3}\int_{10}^{100} \frac{\bar{B}_3(x)\,dx}{x^5} \\
&= \frac{999}{6\cdot 10^6} - 4\int_{10}^{100} \frac{\bar{B}_3(x)\,dx}{x^5}.
\end{aligned}$$

The first term is 1.665×10^{-4} and the second term is much smaller, as can be seen by an alternating series technique similar to the one used to estimate (4). Note first that $B_3(x)$ is a polynomial of degree three which is zero at $x = 0$ and $x = \frac{1}{2}$ [by direct evaluation] and at $x = 1$ [because (6) shows that $B_n(1) = B_n(0)$ for $n \geq 2$]. This accounts for all its zeros and proves that $B_3(x) = x(x - \frac{1}{2})(x - 1)$. Thus it is positive for $0 < x < \frac{1}{2}$ and negative for $\frac{1}{2} < x < 1$. These positive and negative "bumps" are symmetrical because $B_3(1 - x) = (1 - x)(1 - x - \frac{1}{2})(1 - x - 1) = -B_3(x)$, so the graph of $\bar{B}_3(x)$

is a wave consisting of positive bumps on $(n, n+\frac{1}{2})$ and symmetrically negative bumps on $(n+\frac{1}{2}, n+1)$. Since x^{-5} decreases, this shows immediately that

$$0 \le 4\int_{10}^{100} \frac{\bar{B}_3(x)\,dx}{x^5} \le 4\int_{10}^{10.5} \frac{\bar{B}_3(x)\,dx}{x^5}.$$

Now

$$\begin{aligned}
4\int_{10}^{10.5} \frac{\bar{B}_3(x)\,dx}{x^5} &\le \frac{4}{10^5}\int_{10}^{10.5} \bar{B}_3(x)\,dx = \frac{4}{10^5}\int_0^{1/2} B_3(t)\,dt \\
&= \frac{4}{10^5}\left[\frac{1}{4}t^4 - \frac{1}{2}t^3 + \frac{1}{4}t^2\right]\Big|_0^{1/2} = \frac{4}{10^5}\left[\frac{1}{64} - \frac{1}{16} + \frac{1}{16}\right] \\
&= \frac{1}{10^5 \cdot 16} = 6.25 \times 10^{-7}.
\end{aligned}$$

Thus

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

lies in the range

$$0.095215875 \le S \le 0.0952165$$

which gives S to six places.

The integration by parts can of course be carried farther to put (3) in the form

$$\begin{aligned}
(8) \qquad \sum_{n=M}^{N} f(n) = \int_M^N f(x)\,dx &+ \frac{1}{2}[f(M) + f(N)] + \frac{B_2(0)}{2} f'(x)\Big|_M^N \\
&- \frac{B_3(0)}{2\cdot 3} f''(x)\Big|_M^N + \cdots + (-1)^k \frac{B_k(0)}{k!} f^{(k-1)}(x)\Big|_M^N \\
&+ (-1)^{k+1}\frac{1}{k!}\int_M^N \bar{B}_k(x) f^{(k)}(x)\,dx.
\end{aligned}$$

If k is odd, then $\bar{B}_k(x)$ is an oscillating function similar to $\bar{B}_3(x)$ and the integral in this formula can be estimated, provided $f^{(k)}(x)$ is monotone, by an alternating series technique like the one used above. To prove that $\bar{B}_{2\nu+1}(x)$ has this oscillating character, note that the identities

$$\begin{aligned}
\int_x^{x+1} B_n(1-t)\,dt = -\int_{1-x}^{-x} B_n(u)\,du &= \int_{-x}^{-x+1} B_n(u)\,du \\
&= (-x)^n = (-1)^n \int_x^{x+1} B_n(t)\,dt
\end{aligned}$$

and

$$\begin{aligned}
\int_x^{x+(1/2)} B_n(2t)\,dt = \frac{1}{2}\int_{2x}^{2x+1} B_n(u)\,du &= \frac{1}{2}(2x)^n = 2^{n-1}\int_x^{x+1} B_n(t)\,dt \\
&= 2^{n-1}\int_x^{x+(1/2)} [B_n(t) + B_n(t+\tfrac{1}{2})]\,dt
\end{aligned}$$

imply

$$(9)\qquad \begin{aligned} B_n(1-x) &= (-1)^n B_n(x),\\ B_n(2x) &= 2^{n-1}[B_n(x) + B_n(x+\tfrac{1}{2})]. \end{aligned}$$

Thus $B_{2\nu+1}(1-x) = -B_{2\nu+1}(x)$, $B_{2\nu+1}(\frac{1}{2}) = 0$, $B_{2\nu+1}(0) = 2^{2\nu}[B_{2\nu+1}(0) + 0]$, $B_{2\nu+1}(0) = 0$; that is,

$$(10)\qquad B_{2\nu+1}(0) = B_{2\nu+1}(\tfrac{1}{2}) = 0 \qquad (\nu = 1, 2, \ldots).$$

Now there are no zeros of $B_{2\nu+1}(x)$ between 0 and $\frac{1}{2}$ because such a zero would imply two zeros of the derivative $(2\nu+1)B_{2\nu}(x)$ between 0 and $\frac{1}{2}$, which would in turn imply a zero of $(2\nu+1)2\nu B_{2\nu-1}(x)$ and hence a zero of $B_{2\nu-1}(x)$; repeating this process one would ultimately arrive at the conclusion that $B_3(x)$ had a zero between 0 and $\frac{1}{2}$, which it does not; hence neither does $B_{2\nu+1}(x)$. Thus $B_{2\nu+1}(x)$ has one sign on $(0, \frac{1}{2})$; by $B_{2\nu+1}(1-x) = -B_{2\nu+1}(x)$ it has the opposite sign on $(\frac{1}{2}, 1)$. Therefore $\bar{B}_{2\nu+1}(x)$ oscillates as was to be shown.

This also shows, in passing, that many of the terms of (8) are zero, namely, the terms containing $B_{2\nu+1}(0)$. To apply formula (8), one must of course find the values of the constants $B_{2\nu}(0)$. This is accomplished by proving that *the constants $B_{2\nu}(0)$ coincide with the Bernoulli numbers $B_{2\nu}$* defined in Section 1.5. To see this, apply formula (8) in the case $f(x) = e^{-hx}$, $M = 0$, $N = \infty$ to find

$$\begin{aligned} 1 + e^{-h} + e^{-2h} + \cdots &= \int_0^\infty e^{-hx}\,dx + \frac{1}{2} - \frac{B_2(0)}{2}(-h)\\ &\quad + \frac{B_3(0)}{3!}(-h)^2 + \cdots - (-1)^k\frac{B_k(0)}{k!}(-h)^{k-1}\\ &\quad + (-1)^{k+1}(-h)^k\frac{1}{k!}\int_0^\infty \bar{B}_k(x)e^{-hx}\,dx, \end{aligned}$$

$$\begin{aligned} \frac{1}{1-e^{-h}} &= \frac{1}{h} + \frac{1}{2} + \frac{B_2(0)}{2}h + \frac{B_3(0)}{3!}h^2\\ &\quad + \cdots + \frac{B_k(0)}{k!}h^{k-1} - \frac{h^k}{k!}\int_0^\infty \bar{B}_k(x)e^{-hx}\,dx, \end{aligned}$$

$$\begin{aligned} \sum_{n=0}^{\infty}\frac{B_n}{n!}(-h)^n &= \frac{-h}{e^{-h}-1} = h\cdot\frac{1}{1-e^{-h}}\\ &= 1 + \frac{1}{2}h + \frac{B_2(0)}{2}h^2 + \frac{B_3(0)}{3!}h^3 + \cdots\\ &\quad + \frac{B_k(0)}{k!}h^k - \frac{h^{k+1}}{k!}\int_0^\infty \bar{B}_k(x)e^{-hx}\,dx. \end{aligned}$$

This formula is valid for small positive h, and, provided k is odd, the absolute value of the last term is at most $(h^{k+1}/k!)\left|\int_0^{1/2} B_k(t)\,dt\right| \le \text{const}\, h^{k+1}$. Thus the polynomial

$$\sum_{n=0}^{k}[(-1)^n B_n - B_n(0)]\frac{h^n}{n!} = p(h)$$

has the property that $p(h)/h^{k+1}$ is bounded as $h \downarrow 0$, which proves $p(h) \equiv 0$, $B_n(0) \equiv (-1)^n B_n$ for $n \leq k$. Since k was arbitrary and since only even† values of n are at issue, this proves the theorem.

Putting these facts together gives the *Euler–Maclaurin summation formula*

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

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

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

or

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

in which $\bar{B}_k(x) = B_k(x - [x])$. [The two forms of $R_{2\nu}$ are obtained by setting $k = 2\nu$ and $k = 2\nu + 1$, respectively, in (8).]

Continuing with the example of the sum S in (1), the next few terms are

$$\frac{B_4}{4!} \cdot \frac{(-4)(-3)(-2)}{x^5}\Big|_{10}^{100} = -\frac{1}{30}\frac{10^5 - 1}{10^{10}} = -\frac{33333}{10^{11}} = -3.3333 \times 10^{-7}$$

$$\frac{B_6}{6!}\frac{(-6)(-5)\cdots(-2)}{x^7}\Big|_{10}^{100} = \frac{1}{42}\frac{10^7 - 1}{10^{14}} = (2.3809\cdots) \times 10^{-9}$$

$$\frac{B_8}{8!}\frac{(-1)8!}{x^9}\Big|_{10}^{100} = -\frac{1}{30}\frac{10^9 - 1}{10^{18}} = (-3.33\cdots) \times 10^{-11}$$

which gives the approximation 0.095 216 169 017 6 to the value of S. The

0.095 05	−0.000 000 333 33
0.000 166 5	−0. 33 3
0.000 000 002 380 9	−0.000 000 333 363 3
0.095 216 502 380 9	
−0.000 000 333 363 3	
$S \sim$ 0.095 216 169 017 6	

Computation of the approximation to S.

†For odd values of n this gives an alternative proof that $B_3, B_5, B_7, \ldots$ are all zero. See Section 1.6.

magnitude of the error in this approximation is

$$\begin{aligned}\left|\frac{1}{9!}\int_{10}^{100}\bar{B}_9(x)\frac{(-1)10!}{x^{11}}\,dx\right| &\le \frac{1}{10^{11}}\left|\int_0^{1/2} 10B_9(t)\,dt\right| \\ &= 10^{-11}\left|B_{10}\left(\frac{1}{2}\right) - B_{10}(0)\right| \\ &= 10^{-11}\left|B_{10}\left(\frac{1}{2}\right) + B_{10}(0) - 2B_{10}(0)\right| \\ &= 10^{-11}\,|2^{-9}B_{10}(0) - 2B_{10}(0)| \\ &\le 2B_{10}\cdot 10^{-11}.\end{aligned}$$

Rather than use this error estimate directly, however, it is more effective to note that it says that the magnitude of the error cannot be more than about *twice the size of the first term omitted*, and that the same estimate would apply no matter where the series was truncated. Since the terms are still getting smaller—$B_{10} = 5/66$, $B_{12} = -691/2730$ so the next two are about 8 in the thirteenth place and 3 in the fourteenth place—this implies that *the error is of the order of magnitude of the first term omitted* because when this term is included, the error is reduced to an amount much smaller than this term (namely, to an amount comparable to the next term). Thus one can be confident that the error in the above approximation to S is *less than one in the twelfth place*, that is, $S = 0.095\,216\,169\,018 \pm 1$.

It is a general rule of thumb in applying the Euler–Maclaurin summation formula that *as long as the terms are decreasing rapidly in size, the bulk of the error is in the first term omitted.* In order to give a rigorous proof of this fact in specific cases it is not necessary to estimate $|R_{2\nu}|$ in any refined way but merely to give a crude estimate showing that it is of an order of magnitude comparable to the first term omitted at most. Then the error has absolute value at most

$$|R_{2\nu}| = \left|\frac{B_2}{2!}f^{(2\nu-1)}\Big|_N^M + R_{2\nu+2}\right| \le |\text{first term omitted}| + |R_{2\nu+2}|$$

and $|R_{2\nu+2}|$ is comparable to the second term omitted, hence much smaller than the first term omitted.

However, it must be observed that the terms do *not* continue to decrease indefinitely [except for very special functions f such as $f(x) = e^{-hx}$ for small h] and that in fact they ultimately grow without bound. To see this, it suffices to combine Euler's formula

$$\zeta(2\nu) = (2\pi)^{2\nu}(-1)^{\nu+1}B_{2\nu}/2\cdot(2\nu)!$$

[see (2) of Section 1.5] with the trivial observation that $\zeta(2\nu) = 1 + 2^{-2\nu} + 3^{-2\nu} + \cdots$ is only slightly larger than one for ν large; hence

$$B_{2\nu} \sim \pm 2\cdot(2\nu)!(2\pi)^{-2\nu},$$

and in the example the term containing $B_{2\nu}$ is roughly $\pm 2\cdot(2\nu)!(2\pi)^{-2\nu}\cdot 10^{-2\nu-1}$ which decreases quite rapidly at first but which ultimately grows without bound. This shows that there is a limit to the degree of accuracy with which one can evaluate S by extending the above process, and that this limit is roughly determined by the minimum value of $\Pi(x)(20\pi)^{-x}\cdot\frac{1}{5}$ for $x \geq 0$. If for any reason greater accuracy is required, then the first few terms can be summed separately, say $10^{-2} + 11^{-2} + 12^{-2} + 13^{-2} + 14^{-2}$, and the remaining sum evaluated by Euler–Maclaurin summation, which is now much more accurate because the denominators $10^{2\nu+1}$ are replaced by $15^{2\nu+1}$. [This observation is of crucial importance in the evaluation of $\zeta(s)$ by Euler–Maclaurin summation in Section 6.4. After all, the sum S is essentially $\zeta(2)$ except that the first nine terms and all terms past the hundredth are missing.]

In summary, the Euler–Maclaurin summation formula says that

$$\sum_{n=M}^{N} f(n) \sim \int_M^N f(x)\,dx + \frac{1}{2}[f(M) + f(N)] + \sum_{j=1}^{\nu} \frac{B_{2j}}{(2j)!} f^{(2j-1)}(x)\Big|_M^N.$$

In many examples the terms of the series on the right are at first rapidly decreasing in size and the bulk of the error in the approximation is accounted for by the first term omitted. In any case the error is precisely equal to

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

and when $f^{(2\nu+1)}$ is monotone this leads to a simple estimate of $|R_{2\nu}|$ using the fact that $\bar{B}_{2\nu+1}(x)$ alternates in sign.

6.3 EVALUATION OF Π BY EULER–MACLAURIN SUMMATION. STIRLING'S SERIES

To evaluate $\Pi(s)$, it of course suffices to evaluate $\log \Pi(s)$. Now if s is a positive integer, say $s = N$, then $\log \Pi(N) = \sum_1^N \log n$ which, by Euler–Maclaurin summation (with $\nu = 0$), is

$$\int_1^N \log x\,dx + \frac{1}{2}[\log 1 + \log N] + \int_1^N \frac{\bar{B}_1(x)\,dx}{x}.$$

The first integral can be evaluated using $\int \log x\,dx = x\log x - x$. The second integral approaches a limit as $N \to \infty$ (by the alternating series test), so it can be written in the form

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

in which the first term is constant and the second term approaches zero as $N \longrightarrow \infty$. This gives

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

where A is the constant

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

Except for the fact that the constant A must still be evaluated, this gives a simple approximate formula for $\log \Pi(N)$, and it is natural to ask whether there is a similar formula for $\log \Pi(s)$ for other values of s.

As it stands, formula (1) cannot possibly be valid for all real numbers N because the derivative of its right side with respect to N is discontinuous at all integers [because $\bar{B}_1(x)$ is discontinuous]. However, if (1) is rewritten in the form

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

then both sides are well-behaved functions of s for all positive real numbers and, since equality holds whenever s is an integer, it is reasonable to expect that equality will hold for all real $s > 0$. The fact that it does hold follows quite easily from the application of Euler–Maclaurin summation (with $\nu = 0$) to the definition of $\Pi(s)$. Explicitly, from the definition

$$\Pi(s) = \lim_{N \to \infty} \frac{1 \cdot 2 \cdot 3 \cdots N}{(s + 1)(s + 2) \cdots (s + N)} (N + 1)^s$$

of $\Pi(s)$ [see (3) of Section 1.3] it follows that

$$\begin{aligned}
\log \Pi(s) &= \lim_{N \to \infty} \left\{ s \log(N + 1) + \sum_{n=1}^{N} \log n - \sum_{n=1}^{N} \log(s + n) \right\} \\
&= \lim_{N \to \infty} \Bigg\{ s \log(N + 1) + \int_1^N \log x\,dx + \frac{1}{2} \log N + \int_1^N \frac{\bar{B}_1(x)\,dx}{x} \\
&\qquad - \int_1^N \log(s + x)\,dx - \frac{1}{2}[\log(s + 1) + \log(s + N)] \\
&\qquad - \int_1^N \frac{\bar{B}_1(x)\,dx}{s + x} \Bigg\} \\
&= \lim_{N \to \infty} \Bigg\{ s \log(N + 1) + N \log N - N + 1 + \frac{1}{2} \log N + \int_1^N \frac{\bar{B}_1(x)\,dx}{x} \\
&\qquad - (s + N) \log(s + N) + (s + N) + (s + 1) \log(s + 1) \\
&\qquad - (s + 1) - \frac{1}{2} \log(s + 1) - \frac{1}{2} \log(s + N) - \int_1^N \frac{\bar{B}_1(x)\,dx}{s + x} \Bigg\}
\end{aligned}$$

$$
\begin{aligned}
&= \left(s+\frac{1}{2}\right)\log(s+1) + \int_1^\infty \frac{\bar{B}_1(x)\,dx}{x} - \int_1^\infty \frac{\bar{B}_1(x)\,dx}{s+x} \\
&\quad + \lim_{N\to\infty}\left\{s\log(N+1) + \left(N+\frac{1}{2}\right)\log N\right. \\
&\quad \left. - \left(s+N+\frac{1}{2}\right)\log(s+N)\right\} \\
&= \left(s+\frac{1}{2}\right)\log(s+1) + (A-1) - \int_1^\infty \frac{\bar{B}_1(x)\,dx}{s+x} \\
&\quad + \lim_{N\to\infty}\left\{s\log\frac{N+1}{N+s} - \left(N+\frac{1}{2}\right)\log\left(1+\frac{s}{N}\right)\right\} \\
&= \left(s+\frac{1}{2}\right)\log(s+1) + A - 1 - \int_1^\infty \frac{\bar{B}_1(x)\,dx}{s+x} - s.
\end{aligned}
$$

This differs from the right side of (2) by

$$
\begin{aligned}
&\left(s+\frac{1}{2}\right)\log\left(\frac{s+1}{s}\right) - 1 + \int_0^1 \frac{\bar{B}_1(t)\,dt}{s+t} \\
&= \left(s+\frac{1}{2}\right)\log\left(\frac{s+1}{s}\right) - 1 + \int_0^1 \frac{t-\frac{1}{2}}{s+t}\,dt \\
&= \left(s+\frac{1}{2}\right)\log\left(\frac{s+1}{s}\right) - 1 + \int_0^1 \frac{t+s-s-\frac{1}{2}}{s+t}\,dt \\
&= \left(s+\frac{1}{2}\right)\log\left(\frac{s+1}{s}\right) - 1 + \int_0^1 dt - \left(s+\frac{1}{2}\right)\int_0^1 \frac{dt}{s+t} \\
&= 0
\end{aligned}
$$

which shows that (2) is indeed true for all positive real numbers s.

Formula (2) can be combined with the Legendre relation

$$\Pi(2s) = \frac{1}{\pi^{1/2}} 2^{2s}\Pi(s)\Pi\left(s-\frac{1}{2}\right)$$

[see (7) of Section 1.3] to give† the value of the constant A. To this end let (2) be rewritten in the form

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

where

$$r(s) = \exp\left[-\int_0^\infty \frac{\bar{B}_1(t)\,dt}{s+t}\right].$$

†An alternative method of proving $A = \frac{1}{2}\log 2\pi$, not relying on the Legendre relation, is given later in this section.

Then $r(s) \longrightarrow 1$ as $s \longrightarrow \infty$, and the Legendre 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 $s \longrightarrow \infty$ the left side approaches $2^{1/2}e^{1/2}e^{-1/2}\pi^{1/2}\cdot 1 = (2\pi)^{1/2}$, so $A = \frac{1}{2}\log 2\pi$. Thus (2) says

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

or, if the last term is integrated by parts a number of times,

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

where

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

This formula, which is known as *Stirling's series*†, is very effective for finding the approximate numerical value of $\log \Pi(s)$.

For example, consider the case $s = 10$. Then

$$\frac{B_2}{2s} = \frac{1}{6\cdot 2\cdot 10} = \frac{1}{120} = 8.3333\cdots \times 10^{-3},$$
$$\frac{B_4}{4\cdot 3\cdot s^3} = \frac{-1}{30\cdot 4\cdot 3\cdot 10^3} = \frac{-1}{36\cdot 10^4} = -2.7777\cdots \times 10^{-6},$$
$$\frac{B_6}{6\cdot 5\cdot s^5} = \frac{1}{42\cdot 6\cdot 5\cdot 10^5} = \frac{1}{126\cdot 10^6} = 7.936507\cdots \times 10^{-9},$$
$$\frac{B_8}{8\cdot 7\cdot s^7} = \frac{-1}{30\cdot 8\cdot 7\cdot 10^7} = \frac{-1}{168\cdot 10^8} = -5.9523\cdots \times 10^{-11},$$
$$\frac{B_{10}}{10\cdot 9\cdot s^9} = \frac{5}{66\cdot 10\cdot 9\cdot 10^9} = \frac{1}{1188\cdot 10^9} \sim 9 \times 10^{-13}.$$

The terms are still decreasing rapidly and the "rule of thumb" of the previous section would lead one to believe that if the B_{10} term is the first one

†It is named for James Stirling, who published it [S7] in 1730. The integral formula for the remainder $R_{2\nu}$ was published by Stieltjes [S5] in 1889 and does not seem to have been known, or at least used, earlier than that.

omitted, then the error will not be much larger than 9×10^{-13}, so the answer will be correct to 12 places. Now in fact

$$\begin{aligned}|R_{10}| &= \left|\int_0^\infty \frac{\bar{B}_{11}(x)\,dx}{11\cdot(10+x)^{11}}\right| \le \left|\int_0^{1/2} \frac{B_{11}(x)\,dx}{11\cdot(10+x)^{11}}\right| \\ &\le \frac{1}{12\cdot 11\cdot 10^{11}}\left|\int_0^{1/2} 12B_{11}(x)\,dx\right| \\ &= \frac{1}{12\cdot 11\cdot 10^{11}}\left|B_{12}\left(\frac{1}{2}\right) - B_{12}(0)\right| = \frac{|B_{12}|(2-2^{-11})}{12\cdot 11\cdot 10^{11}} \\ &\le \frac{2\cdot 691}{12\cdot 11\cdot 10^{11}\cdot 2730},\end{aligned}$$

so $|R_{10}|$ is very much smaller than the B_{10} term, and hence $|R_8| \sim 9 \times 10^{-13}$ as expected. Thus $\log \Pi(10) \sim 15.10441\,25730\,7470$ is accurate to 12 places.

(10.5) $\log 10 =$	24.17714 34764 3748
$-10 =$	$-10.$
$+\frac{1}{2}\log \pi =$	+0.57236 49429 2470
$+\frac{1}{2}\log 2 =$	+0.34657 35902 7997
B_2 term $=$	+0.00833 33333 3333
B_4 term $=$	−0.00000 27777 7777
B_6 term $=$	+0.00000 00079 3651
B_8 term $=$	−0.00000 00000 5952
$\log \Pi(10) \sim$	15.10441 25730 7470

Computation of the approximation to $\log \Pi(10)$.

Of course, if $s > 10$, then the terms of Stirling's series decrease even faster at first and it is even easier to compute $\log \Pi(s)$ with 10- or 12-place accuracy. In fact, Stirling's series is so effective a means of computation that one tends to forget that the series does not converge and that there is a limit to the accuracy with which $\log \Pi(s)$ can be computed using it. Nonetheless, the terms of Stirling's series do ultimately grow without bound as $\nu \to \infty$, and one cannot expect to reduce the error in the approximation to less than the size of the smallest term of the series. If it is desired to compute $\log \Pi(s)$ with greater accuracy than is possible with Stirling's series, then the formula

$$\begin{aligned}\log \Pi(s) = \log \Pi(s+N) &- \log(s+1) \\ &- \log(s+2) - \cdots - \log(s+N)\end{aligned}$$

can be used. Given $\epsilon > 0$ there is an N such that Stirling's series can be used to compute $\log \Pi(s+N)$ with an error of less than ϵ; since the other logarithms can then be computed by elementary means, this makes possible the evaluation of $\log \Pi(s)$ with any prescribed degree of accuracy. In the numerical analysis of the roots ρ it will not be necessary to use this technique, however, because Stirling's series itself gives the needed values with sufficient accuracy.

Once $\log \Pi(s)$ is found, $\Pi(s)$ can of course be found simply by exponentiating. Note that if $\log \Pi(s)$ is found to 12 decimal places, then $\Pi(s)$ is known to within a *factor* of $\exp(\pm 10^{-12}) \sim 1 \pm 10^{-12}$; so it is the *relative* error which is small, that is, the error divided by the value is less than 10^{-12}. Since $\Pi(s)$ is very large for large s, it is well to keep in mind in evaluating $\Pi(s)$ using Stirling's series that a small relative error may still mean a large absolute error. However, in the numerical analysis of the roots ρ only $\log \Pi(s)$—and in fact only $\operatorname{Im} \log \Pi(s)$—will need to be evaluated, so these considerations will not be necessary.

What *will* be necessary 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 numbers other than the negative reals and zero. Then all terms of Stirling's series (3) are defined throughout the slit plane and are analytic functions of s. (This is obvious for all terms except the integral for R_0. However, as will be shown below, this integral too is convergent for all s in the slit plane.) Since (3) is true for positive real s, the theory of analytic continuation implies that it is true throughout the slit plane—in Riemann's terminology formula (3) for $\log \Pi(s)$ remains valid throughout the slit plane. However, the alternating series method of estimating $|R_{2\nu}|$ cannot be used when s is not real, so some other method of estimating $|R_{2\nu}|$ is needed if Stirling's series is to be used to compute $\log \Pi(s)$ for complex s. The following estimate was given by Stieltjes [S5]:

The objective is to show that the error at any stage is comparable in magnitude to the first term omitted. To this end, let the $B_{2\nu}$ term be the first term omitted and consider the resulting error

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

The function $B_{2\nu} - \bar{B}_{2\nu}(x)$ is an antiderivative of $-2\nu\bar{B}_{2\nu-1}(x)$ which is zero at $x = 0$; hence by integration by parts

$$R_{2\nu-2} = \int_0^\infty \frac{[B_{2\nu} - \bar{B}_{2\nu}(x)]\,dx}{2\nu(s+x)^{2\nu}}.$$

[This integration by parts can be justified, even in the case $\nu = 1$ where $\bar{B}_{2\nu-1}(x)$ is discontinuous, by writing the integral for $R_{2\nu-2}$ as a sum over n of

Riemann integrals, as in the previous section.] Thus

$$|R_{2\nu-2}| \leq \int_0^\infty \frac{|B_{2\nu} - \bar{B}_{2\nu}(x)|\,dx}{2\nu|s+x|^{2\nu}}.$$

Now $B_{2\nu} - B_{2\nu}(x)$ is zero at $x = 0$ and has only one extremum in the interval $0 < x < 1$, namely, at $x = \frac{1}{2}$ where its derivative $-2\nu B_{2\nu-1}(x)$ is zero. This implies that $B_{2\nu} - \bar{B}_{2\nu}(x)$ never changes sign. Since $\bar{B}_{2\nu}(x)$ has zeros—namely, at the extrema of $\bar{B}_{2\nu+1}$—the sign of $B_{2\nu} - \bar{B}_{2\nu}(x)$ is always the same as the sign of $B_{2\nu}$, which by Euler's formula for $\zeta(2\nu)$ [(2) of Section 1.5] is $(-1)^{\nu+1}$. Therefore the numerator of the above integral can be rewritten

$$|B_{2\nu} - \bar{B}_{2\nu}(x)| = (-1)^{\nu+1}[B_{2\nu} - \bar{B}_{2\nu}(x)].$$

On the other hand, it is a simple calculus problem to show that $|s + x|(|s| + x)^{-1}$ for $s = re^{i\theta}$ in the slit plane $\{-\pi < \theta < \pi\}$ assumes its minimum value for $x \geq 0$ at $x = |s|$ where it is $\cos(\theta/2)$. Thus

$$\frac{1}{|s+x|} = \frac{1}{|s|+x} \cdot \frac{|s|+x}{|s+x|} \leq \frac{1}{(|s|+x)\cos(\theta/2)}$$

and

$$\begin{aligned}
|R_{2\nu-2}| &\leq \int_0^\infty \frac{(-1)^{\nu+1}[B_{2\nu} - \bar{B}_{2\nu}(x)]\,dx}{2\nu\cos^{2\nu}(\theta/2)(|s|+x)^{2\nu}} \\
&= \int_0^\infty \frac{(-1)^{\nu+1}B_{2\nu}\,dx}{2\nu\cos^{2\nu}(\theta/2)(|s|+x)^{2\nu}} \\
&\quad - \int_0^\infty \frac{(-1)^{\nu+1}\bar{B}_{2\nu}(x)\,dx}{2\nu\cos^{2\nu}(\theta/2)(|s|+x)^{2\nu}} \\
&= \frac{1}{\cos^{2\nu}(\theta/2)} \cdot \frac{|B_{2\nu}|}{2\nu(2\nu-1)|s|^{2\nu-1}} \\
&\quad - \frac{1}{\cos^{2\nu}(\theta/2)} \int_0^\infty \frac{(-1)^{\nu+1}\bar{B}_{2\nu+1}(x)\,dx}{(2\nu+1)(|s|+x)^{2\nu+1}}.
\end{aligned}$$

By the alternating series method, the second integral is easily seen to have the same sign as $(-1)^{\nu+1}\bar{B}_{2\nu+1}(x)$ on $\{0 < x < \frac{1}{2}\}$. Since this function starts at $x = 0$ with the value zero and the derivative $(-1)^{\nu+1}(2\nu + 1)B_{2\nu} > 0$, this sign is $+$ and the inequality becomes stronger if the last term is deleted

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

which is the desired inequality. In words, *if the $B_{2\nu}$ term 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 the first term omitted.*

In the special case $\nu = 1$, $\operatorname{Re} s \geq 0$, $\cos(\theta/2) \geq \sqrt{2}/2$, this gives the estimate used in Section 3.4, namely, that the magnitude of the error in the approximation $\log \Pi(s/2) \sim (s + \frac{1}{2}) \log s - s + \frac{1}{2} \log 2\pi$ is at most $(6|s|)^{-1}$ in the halfplane $\operatorname{Re} s \geq 0$. More generally, it shows that if s is a real number $s > 0$, the magnitude of the error is at most the magnitude of the first term omitted (each new term overshoots the mark and the true value lies between any two consecutive partial sums of Stirling's series) and if s is any complex number in the slit plane, then the magnitude of the error is *comparable* to the magnitude of the first term omitted unless s is quite near the negative real axis. This implies that, unless s is near the negative real axis, one is reasonably safe in using the rule of thumb that when the terms are rapidly decreasing in magnitude, the first term omitted accounts for the bulk of the error (because when it is included, the error is reduced to the next lower order of magnitude).

The constant A in Stirling's formula can be evaluated quite easily by applying Stirling's formula on the imaginary axis and combining the result with the estimate of Re $\log \Pi$ on the imaginary axis which follows from

$$\sin \pi s = \pi s/\Pi(s)\Pi(-s)$$

[see (6) of Section 1.3]. Since Π is real on the real axis, the reflection principle implies $\Pi(\bar{s}) = \overline{\Pi(s)}$, and with $s = it$, the above gives

$$|\Pi(it)|^2 = \frac{\pi it}{\sin \pi it} = \frac{2\pi t}{e^{\pi t} - e^{-\pi t}},$$

$$2 \log |\Pi(it)| = \log 2\pi + \log t - \log e^{\pi t} - \log(1 - e^{-2\pi t}),$$

$$\operatorname{Re} \log \Pi(it) = \frac{1}{2} \log 2\pi + \frac{1}{2} \log t - \frac{\pi t}{2} - \frac{1}{2} \log(1 - e^{-2\pi t}).$$

On the other hand by Stirling's formula (2)

$$\operatorname{Re} \log \Pi(it) = \operatorname{Re}\left\{\left(it + \frac{1}{2}\right) \log it - it + A - \int_0^\infty \frac{\bar{B}_1(u)\, du}{u + it}\right\}$$

$$= \frac{1}{2} \log t - t\frac{\pi}{2} + A - \int_0^\infty \frac{u\bar{B}_1(u)\, du}{u^2 + t^2};$$

hence

$$A = \frac{1}{2} \log 2\pi - \frac{1}{2} \log(1 - e^{-2\pi t}) + \int_0^\infty \frac{u\bar{B}_1(u)\, du}{u^2 + t^2}$$

and the desired result $A = \frac{1}{2} \log 2\pi$ follows by taking the limit as $t \to \infty$.

The derivative of Stirling's series is the series

$$\frac{\Pi'(s)}{\Pi(s)} = \log s + \frac{1}{2s} - \frac{B_2}{2s^2} - \frac{B_4}{4s^4} - \cdots - \frac{B_{2\nu}}{2\nu s^{2\nu}} + R'_{2\nu}, \tag{4}$$

where

$$R'_{2\nu} = \int_0^\infty \frac{\bar{B}_{2\nu}(x)\, dx}{(s + x)^{2\nu+1}} = \int_0^\infty \frac{\bar{B}_{2\nu+1}(x)\, dx}{(s + x)^{2\nu+2}}.$$

This gives a precise form of the estimate $\Pi'(s)/\Pi(s) \sim \log s$ which was used in de la Vallée Poussin's proof in Section 5.2. Specifically, to prove that there is a $K > 0$ such that

$$\operatorname{Re} \frac{\Pi'[(\sigma + it)/2]}{\Pi[(\sigma + it)/2]} \leq 2 \log t$$

in the region $1 \le \sigma \le 2$, $t \ge K$ as was claimed in Section 5.2, it suffices to estimate R_0' to find

$$|R_0'| \le \frac{1}{\cos^3(\theta/2)} \cdot \left|\frac{B_2}{2s^2}\right|,$$

$$\left|\frac{\Pi'(s)}{\Pi(s)} - \log s\right| \le \frac{1}{2|s|} + \frac{B_2}{\cos^3(\theta/2)2|s|^2}.$$

For s in the halfplane $\operatorname{Re} s \ge 0$ and for $|s|$ sufficiently large, this gives

$$\left|\operatorname{Re}\frac{\Pi'(s)}{\Pi(s)} - \operatorname{Re}\log s\right| \le \frac{1}{|s|},$$

$$\operatorname{Re}\frac{\Pi'[(\sigma+it)/2]}{\Pi[(\sigma+it)/2]} \le \log\left|\frac{\sigma+it}{2}\right| + \frac{1}{|s|}$$

from which the desired inequality follows.

6.4 EVALUATION OF ζ BY EULER–MACLAURIN SUMMATION

Euler–Maclaurin summation applied directly to the series $\zeta(s) = \sum_1^\infty n^{-s}$ ($\operatorname{Re} s \ge 1$) does not give a workable method of evaluating $\zeta(s)$ because the remainders are not at all small. [This is the case $N = 1$ of formula (1) below.] However, if Euler–Maclaurin is applied instead to the series $\sum_{n=N}^\infty n^{-s}$, it gives a quite workable means of approximating numerically the sum of this series and hence, since the terms $\sum_{n=1}^{N-1} n^{-s}$ can be summed directly, a workable means of evaluating $\zeta(s)$. Explicitly, if $\operatorname{Re} s > 1$, then

$$\sum_{n=1}^{\infty} n^{-s} - \sum_{n=1}^{N-1} n^{-s} = \sum_{n=N}^{\infty} n^{-s},$$

$$\zeta(s) - \sum_{n=1}^{N-1} n^{-s} = \int_N^\infty x^{-s}\,dx + \tfrac{1}{2}N^{-s} + \int_N^\infty \bar{B}_1(x)(-s)x^{-s-1}\,dx,$$

$$\zeta(s) = \sum_{n=1}^{N-1} n^{-s} + \frac{N^{1-s}}{s-1} + \frac{1}{2}N^{-s} + \frac{B_2}{2}sN^{-s-1} + \cdots + \frac{B_{2\nu}}{(2\nu)!}s(s+1)\cdots(s+2\nu-2)N^{-s-2\nu+1} + R_{2\nu}, \tag{1}$$

where

$$R_{2\nu} = -\frac{s(s+1)\cdots(s+2\nu-1)}{(2\nu)!}\int_N^\infty \bar{B}_{2\nu}(x)x^{-s-2\nu}\,dx$$
$$= -\frac{s(s+1)\cdots(s+2\nu)}{(2\nu+1)!}\int_N^\infty \bar{B}_{2\nu+1}(x)x^{-s-2\nu-1}\,dx.$$

If N is at all large, say N is about the same size as $|s|$, then the terms of the series (1) decrease quite rapidly at first and it is natural to expect that the remainder $R_{2\nu}$ will be quite small. The same method by which Stieltjes estimated the remainder in Stirling's series can be applied to estimate the remainder $R_{2\nu}$ above. It gives

$$\begin{aligned}
|R_{2\nu-2}| &= \left|\frac{s(s+1)\cdots(s+2\nu-2)}{(2\nu-1)!}\int_N^\infty \bar{B}_{2\nu-1}(x)x^{-s-2\nu+1}\,dx\right| \\
&= \left|\frac{s(s+1)\cdots(s+2\nu-1)}{(2\nu)!}\int_N^\infty [B_{2\nu}-\bar{B}_{2\nu}(x)]x^{-s-2\nu}\,dx\right| \\
&\le \left|\frac{s(s+1)\cdots(s+2\nu-1)}{(2\nu)!}\right|\int_N^\infty (-1)^{\nu+1}[B_{2\nu}-\bar{B}_{2\nu}(x)]x^{-\sigma-2\nu}\,dx \\
&= \left|\frac{s(s+1)\cdots(s+2\nu-1)}{(2\nu)!}\right||B_{2\nu}|\int_N^\infty x^{-\sigma-2\nu}\,dx \\
&\quad -\left|\frac{s(s+1)\cdots(s+2\nu-1)}{(2\nu)!}\right|\int_N^\infty \frac{(-1)^{\nu+1}\bar{B}_{2\nu+1}(x)}{(2\nu+1)} \\
&\quad \times(\sigma+2\nu)x^{-\sigma-2\nu-1}\,dx \\
&\le \left|\frac{s(s+1)\cdots(s+2\nu-1)B_{2\nu}N^{-\sigma-2\nu+1}}{(2\nu)!(\sigma+2\nu-1)}\right| \\
&= \left|\frac{s+2\nu-1}{\sigma+2\nu-1}\right||B_{2\nu}\text{ term of (1)}|,
\end{aligned}$$

where $\sigma = \operatorname{Re} s$. In words, *if the $B_{2\nu}$ term is the first term omitted, then the magnitude of the remainder in the series* (1) *is at most* $|s+2\nu-1|(\sigma+2\nu-1)^{-1}$ *times the magnitude of the first term omitted.* This estimate is due to Backlund [B2]. In particular, if s is real, the remainder is less than the first term omitted, every term overshoots, and the actual value always lies between two consecutive partial sums of the series (1).

Although formula (1) is derived from the formula $\zeta(s) = \Sigma n^{-s}$ which is valid only for $\operatorname{Re} s > 1$, it obviously "remains valid," in Riemann's terminology, as long as the integral for $R_{2\nu}$ converges, which is true throughout the halfplane $\operatorname{Re}(s + 2\nu + 1) > 1$. Since ν is arbitrary, this gives an alternate proof of the fact that $\zeta(s)$ can be continued analytically throughout the s-plane with just one simple pole at $s = 1$ and no other singularities.

For some idea of how formula (1) works in actual practice, consider the case $s = 2$. A good way to proceed is to compute the first several numbers in the sequence $s(s+1)\cdots(s+2\nu-2)B_{2\nu}/(2\nu)!$ and to see how large N must be in order to make the terms of the series (1) decrease rapidly in size. Now

$$\frac{B_2}{2}\cdot 2 = \frac{1}{6} = 0.16666\ldots,$$

$$\frac{B_4}{4!}\cdot 2\cdot 3\cdot 4 = -\frac{1}{30} = -0.03333\ldots,$$

$$\frac{B_6}{6!}\cdot 2\cdot 3\cdot 4\cdot 5\cdot 6 = \frac{1}{42} = 0.0238095\ldots.$$

$1^{-2} =$	1.000 000 00
$2^{-2} =$	0.250 000 00
$3^{-2} =$	0.111 111 11
$4^{-2} =$	0.062 500 00
$5^{-1}(2-1)^{-1} =$	0.200 000 00
$\frac{1}{2}5^{-2} =$	0.020 000 00
B_2 term $=$	0.001 333 33
B_4 term $=$	−0.000 010 66
$\zeta(2) \sim$	1.644 933 78

Computation of approximation to $\zeta(2)$.

With $N = 5$ the last term is divided by $5^7 > 70{,}000$ so it is less than about 3 in the seventh place. Thus the approximation $\zeta(2) \sim 1.644\,933\,78$ is correct to six decimal places. For $s = \frac{1}{2}$ the terms decrease even more rapidly and with N only equal to 4 the B_6 term is just

$$\frac{B_6}{6!}\cdot\left(\frac{1}{2}\right)\left(\frac{3}{2}\right)\left(\frac{5}{2}\right)\left(\frac{7}{2}\right)\left(\frac{9}{2}\right)4^{-11/2} = \frac{1}{2^{21}} = \frac{1}{2}(2^{-10})^2 < \frac{1}{2}(10^{-3})^2,$$

so it does not affect the sixth decimal place and the approximation† $\zeta(\frac{1}{2}) \sim$ 1.460 354 96 is correct to six decimal places.

$1^{-1/2} =$	1.000 000 00
$2^{-1/2} =$	0.707 106 78
$3^{-1/2} =$	0.577 350 27
$4^{1/2}(\frac{1}{2}-1)^{-1} =$	−4.000 000 00
$\frac{1}{2}4^{-1/2} =$	0.250 000 00
B_2 term $=$	0.005 208 33
B_4 term $=$	−0.000 020 34
$\zeta(\frac{1}{2}) \sim$	−1.460 354 96

Computation of approximation to $\zeta(\frac{1}{2})$.

Consider finally a case in which s is not real, the case $s = \frac{1}{2} + 18i$. Since $|s|$ is considerably larger in this case than in the two previous ones, it is clear that it will be necessary to use a much larger value of N in order to achieve comparable accuracy. On the other hand, the numbers $2^{-s}, 3^{-s}, \ldots$ are quite a bit more difficult to compute when s is complex (since $n^{-s} = n^{-1/2}e^{-i18\log n} = n^{-1/2}[\cos(18\log n) - i\sin(18\log n)]$ each one involves computing a square root, a logarithm, and two trigonometric functions), so this involves a great deal of computation. Rather than carry through all this computation, it will

†The square roots $(0.5)^{1/2}$, $(0.333\ldots)^{1/2}$ can be computed very easily using the usual iteration $x_{n+1} = \frac{1}{2}(x_n + Ax_n^{-1})$ for $A^{1/2}$.

be more illustrative of the technique to settle for less accuracy and to use a smaller value of N. Since $4^{-s} = (2^{-s})^2$ and $6^{-s} = 2^{-s}\cdot 3^{-s}$, the three values 2^{-s}, 3^{-s}, and 5^{-s} are the only values of n^{-s} which need to be computed in order to use (1) with $N = 6$. For this reason, the value $N = 6$ will be used in the computation below.

The first step is to estimate the size of the $B_{2\nu}$ terms in order to determine the degree of accuracy with which the calculations should be carried out. The B_2 term has modulus about $\frac{1}{2}|B_2|\cdot 18\cdot 6^{-3/2} = (2\cdot 2\cdot\sqrt{6})^{-1} \sim 0.1$, the B_4 term modulus about $18\cdot 18\cdot 18/24\cdot 30\cdot 6^{7/2} = 3/8\cdot 10\sqrt{6} \sim 3/196 \sim 0.015$, and the B_6 term modulus about $18\cdot 18\cdot 18\cdot 18\cdot 20/6!\cdot 42\cdot 6^{11/2} = (2^3\cdot 14\cdot\sqrt{6})^{-1} \sim 1/270 \sim 0.0037$. The modulus of the B_8 term is about 0.0037 times

$$\left|\frac{B_8}{B_6\cdot 8\cdot 7}\cdot\left(\frac{11}{2}+18i\right)\left(\frac{13}{2}+18i\right)6^{-2}\right| \sim \frac{42}{30\cdot 8\cdot 7\cdot 6\cdot 6}|6+18i|^2 = \frac{1}{4},$$

so it is about 9 in the fourth place. Then the modulus of the B_{10} term is about 0.0009 times

$$\begin{aligned}\left|\frac{B_{10}}{B_8\cdot 10\cdot 9}\cdot\left(\frac{15}{2}+18i\right)\left(\frac{17}{2}+18i\right)6^{-2}\right| &\sim \frac{5\cdot 30(8^2+18^2)}{66\cdot 10\cdot 9\cdot 6^2}\\ &\sim \frac{5^2\cdot 2^2(4^2+9^2)}{11\cdot 10\cdot 9\cdot 6^2} \sim \frac{100\cdot 97}{1{,}000\cdot 36}\\ &\sim 0.27,\end{aligned}$$

so it is less than 3 in the fourth place. Thus, by Backlund's estimate of the remainder, if the B_{10} term is the first one omitted, the error is less than $|s + 9|$ $(\frac{1}{2} + 9)^{-1}\cdot 3\cdot 10^{-4} \sim |1 + 2i|\cdot 3\cdot 10^{-4} < 7\cdot 10^{-4}$ so the answer is correct to three decimal places at least. The terms are now decreasing fairly slowly; two more terms would be required to obtain one more place, so it is reasonable to quit with the B_8 term. [If more than three-place accuracy were required, the easiest way to achieve it would probably be to compute 7^{-s}, after which $8^{-s} = 2^{-s}\cdot 4^{-s}$, $9^{-s} = (3^{-s})^2$, $10^{-s} = 2^{-s}\cdot 5^{-s}$ are easy and one can use $N = 10$ in (1).] Therefore the calculations will be carried out to five places with the intention of retaining three places in the final answer.

To compute 2^{-s} $(s = \frac{1}{2} + 18i)$ with five-place accuracy, one must have accurate values of $\log 2$ and π, say $\log 2 = 0.693\,147\,18$ and $\pi = 3.141\,592\,65$. Then $18\log 2 = 4\pi - \theta$, where θ is 0.08972 to five places. The power series for $\cos\theta$ and $\sin\theta$ then give $\cos\theta = 0.99598$, $\sin\theta = 0.08960$ which, combined with the value $2^{-1/2} = 0.707\,11$ found above, gives $2^{-s} = (0.704\,27) + (0.063\,36)i$. Similarly, using accurate values of $\log 3$ and π, one can find $18\log 3 = 6\pi + (\pi/3) - \theta$ where $\theta = 0.12174$ to five places, from which

$$\begin{aligned}3^{-s} = 3^{-1/2}e^{-i\pi/3}e^{i\theta} &= \frac{1}{\sqrt{3}}\left(\frac{1}{2}-\frac{\sqrt{3}}{2}i\right)(\cos\theta + i\sin\theta)\\ &= 0.34726 - 0.46124i\end{aligned}$$

can be computed. Finally, $18 \log 5 = 9\pi + (\pi/4) - \theta$, where $\theta = 0.08985$ so that

$$5^{-s} = -\frac{1}{\sqrt{5}}\left(\frac{1}{\sqrt{2}} - \frac{i}{\sqrt{2}}\right)(\cos\theta + i\sin\theta) = -0.34333 + 0.28657i.$$

Using these values one can then compute $4^{-s} = 0.49199 + 0.08924i$ and $6^{-s} = 0.27379 - 0.30284i$ with (almost) five-place accuracy. Now

$$\frac{B_2}{2}s\cdot 6^{-s-1} = \left(\frac{1}{144} + \frac{1}{4}i\right)6^{-s} = 0.07761 + 0.06634i,$$

$$\begin{aligned}\frac{B_4}{4!}s(s+1)(s+2)6^{-s-3} &= -\frac{(\frac{1}{2} + 18i)(\frac{3}{2} + 18i)(\frac{5}{2} + 18i)}{30\cdot 24\cdot 6^3}6^{-s} \\ &= \frac{1456\frac{1}{8} + 5728\frac{1}{2}i}{720\cdot 6^3}\cdot 6^{-s} \\ &= 0.01372 + 0.00725i.\end{aligned}$$

The B_6 term is the B_4 term times

$$\frac{B_6(\frac{7}{2} + 18i)(\frac{9}{2} + 18i)}{B_4\cdot 6\cdot 5\cdot 6^2} = \frac{308\frac{1}{4} - 144i}{1512} = 0.20387 - 0.09524i$$

so it is $0.00349 + 0.00017i$. Similarly the B_8 term is the B_6 term times

$$\frac{B_8(\frac{11}{2} + 18i)(\frac{13}{2} + 18i)}{B_6\cdot 8\cdot 7\cdot 6^2} = \frac{288\frac{1}{4} - 216i}{1440}$$

which gives $0.00072 - 0.00053i$ as the value of the B_8 term. Adding these values up then gives $\zeta(\frac{1}{2} + 18i) \sim 2.329\,22 - 0.188\,65i$ as the value of $\zeta(\frac{1}{2} + 18i)$ to three decimal places.

$1^{-s} =$	$1.000\,00$
$2^{-s} =$	$+0.704\,27 + 0.063\,36i$
$3^{-s} =$	$+0.347\,26 - 0.461\,24i$
$4^{-s} =$	$+0.491\,99 + 0.089\,24i$
$5^{-s} =$	$-0.343\,33 + 0.286\,57i$
$6^{1-s}(s-1)^{-1} =$	$-0.103\,40 - 0.088\,39i$
$\frac{1}{2}6^{-s} =$	$+0.136\,89 - 0.151\,42i$
B_2 term $=$	$+0.077\,61 + 0.066\,34i$
B_4 term $=$	$+0.013\,72 + 0.007\,25i$
B_6 term $=$	$+0.003\,49 + 0.000\,17i$
B_8 term $=$	$+0.000\,72 - 0.000\,53i$
$\zeta(\frac{1}{2} + 18i) \sim$	$2.329\,22 - 0.188\,65i$

Computation of approximation to $\zeta(\frac{1}{2} + 18i)$.

6.5 TECHNIQUES FOR LOCATING ROOTS ON THE LINE

The roots ρ are by definition the zeros of the function $\xi(s) = \Pi(s/2)\pi^{-s/2}(s-1)\zeta(s)$. For any given s, the value of $\xi(s)$ can be computed to any prescribed degree of accuracy by combining the techniques of the preceding two sections. Since $\xi(s)$ is *real valued* on the line $\operatorname{Re} s = \frac{1}{2}$, it can be shown to have zeros on the line by showing that it *changes sign*. This, in a nutshell, is the method by which roots ρ on the line $\operatorname{Re} s = \frac{1}{2}$ will be located in this section.

Consider, then, the problem of determining the sign of $\xi(\frac{1}{2} + it)$. If this function of t is rewritten in the form

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

(where $s = \frac{1}{2} + it$), then the determination of its sign can be simplified by the observation that the factor in the first set of brackets is a negative real number; hence that the sign of $\xi(\frac{1}{2} + it)$ is opposite to the sign of the factor in the second set of brackets. The standard notation for this second factor is $Z(t)$, that is,

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

where $\vartheta(t)$ is defined by

$$\vartheta(t) = \operatorname{Im} \log \Pi\left(\frac{it}{2} - \frac{3}{4}\right) - \frac{t}{2}\log \pi.$$

If $\vartheta(t)$ and $Z(t)$ are so defined, then *the sign of* $\xi(\frac{1}{2} + it)$ *is opposite to the sign*† *of* $Z(t)$. Thus, to determine the sign of $\xi(\frac{1}{2} + it)$ it suffices to compute $\vartheta(t)$, $\zeta(\frac{1}{2} + it)$ by the methods of the preceding two sections and to combine them to find $Z(t)$.

The computation of $\vartheta(t)$ can be simplified as follows:

$$\begin{aligned}\vartheta(t) &= \operatorname{Im}\left[\log \Pi\left(\frac{it}{2} + \frac{1}{4}\right) - \log\left(\frac{it}{2} + \frac{1}{4}\right)\right] - \frac{t}{2}\log \pi \\ &= \operatorname{Im}\left[\left(\frac{it}{2} - \frac{1}{4}\right)\log\left(\frac{it}{2} + \frac{1}{4}\right) - \left(\frac{it}{2} + \frac{1}{4}\right) + \frac{1}{2}\log 2\pi\right. \\ &\quad \left. + \frac{1}{12\left(\frac{it}{2} + \frac{1}{4}\right)} - \frac{1}{360\left(\frac{it}{2} + \frac{1}{4}\right)^3} + \cdots\right] - \frac{t}{2}\log \pi\end{aligned}$$

†In particular, $Z(t)$ is real when, of course, t is real.

$$
\begin{aligned}
&= \frac{t}{2}\operatorname{Re}\log\left(\frac{it}{2}+\frac{1}{4}\right) - \frac{1}{4}\operatorname{Im}\log\left(\frac{it}{2}+\frac{1}{4}\right) - \frac{t}{2} \\
&\quad + \frac{-\frac{t}{2}}{12\left(\frac{t^2}{4}+\frac{1}{16}\right)} - \frac{\operatorname{Im}\left(-\frac{it}{2}+\frac{1}{4}\right)^3}{360\left(\frac{t^2}{4}+\frac{1}{16}\right)^3} + \cdots - \frac{t}{2}\log\pi \\
&= \frac{t}{2}\log\left[\left(\frac{t}{2}\right)^2\left(1+\frac{1}{4t^2}\right)\right]^{1/2} - \frac{1}{4}\left[\frac{\pi}{2} - \operatorname{Arctan}\left(\frac{1}{4}\Big/\frac{t}{2}\right)\right] - \frac{t}{2} \\
&\quad - \frac{1}{6t\left(1+\frac{1}{4t^2}\right)} - \frac{\frac{t^3}{8}+3\left(-\frac{t}{2}\right)\left(\frac{1}{4}\right)^2}{360\left(\frac{t^2}{4}\right)^3\left(1+\frac{1}{4t^2}\right)^3} + \cdots - \frac{t}{2}\log\pi \\
&= \frac{t}{2}\log\frac{t}{2} + \frac{t}{4}\log\left(1+\frac{1}{4t^2}\right) - \frac{\pi}{8} + \frac{1}{4}\operatorname{Arctan}\left(\frac{1}{2t}\right) \\
&\quad - \frac{t}{2} - \frac{1}{6t}\left(1+\frac{1}{4t^2}\right)^{-1} - \frac{1}{45t^3}\left(1+\frac{1}{4t^2}\right)^{-3} \\
&\quad + \frac{1}{60t^5}\left(1+\frac{1}{4t^2}\right)^{-3} + \cdots - \frac{t}{2}\log\pi \\
&= \frac{t}{2}\log\frac{t}{2\pi} + \frac{t}{4}\left[\frac{1}{4t^2} - \frac{1}{2}\left(\frac{1}{4t^2}\right)^2 + \cdots\right] \\
&\quad - \frac{\pi}{8} + \frac{1}{4}\left[\left(\frac{1}{2t}\right) - \frac{1}{3}\left(\frac{1}{2t}\right)^3 + \cdots\right] \\
&\quad - \frac{t}{2} - \frac{1}{6t}\left[1 - \frac{1}{4t^2} + \cdots\right] - \frac{1}{45t^3}\left[1 - \frac{3}{4t^2} + \cdots\right] \\
&\quad + \frac{1}{60t^5}\left(1+\frac{1}{4t^2}\right)^{-3} + \cdots.
\end{aligned}
$$

This gives finally

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

Since the terms decrease very rapidly for t at all large and since the error is comparable to the first term omitted, it is clear that the error in the approximation

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

is very slight. Specifically, the error involved in the above use of Stirling's series is less than

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

and the errors resulting from truncating the alternating series are less than the first term omitted, which gives a total error of less than

$$\frac{t}{4}\cdot\frac{1}{3}\left(\frac{1}{4t^2}\right)^3+\frac{1}{4}\cdot\frac{1}{5}\left(\frac{1}{2t}\right)^5+\frac{1}{6t}\left(\frac{1}{4t^2}\right)^2+\frac{1}{45t^3}\cdot\frac{1}{60t^5}<\frac{1}{t^5},$$

so the total error in the approximation (2) is comfortably less than

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

The second term in this estimate is very crude and could be much improved by using more terms of Stirling's series, finding further terms of the series (1), and estimating the error in terms of t^{-7} or t^{-9} to show that the first term $7/5760t^3$ contains the bulk of the error when t is at all large. However, this form of the estimate is quite adequate for the numerical analysis of the roots ρ.

Thus to find the sign of $\xi(\frac{1}{2}+18i)$ one can simply compute

$$\begin{aligned}\vartheta(18) &\sim 9\log\frac{9}{\pi}-9-\frac{\pi}{8}+\frac{1}{48\cdot 18}\\ &= 9.472452-9-0.392699+0.001158\\ &= 0.080911\end{aligned}$$

and combine it with the value of $\zeta(\frac{1}{2}+18i)$ computed in the previous section to find that

$$Z(18)=e^{0.0809i}(2.329-0.189i)=2.337+0.000i$$

is positive and that $\xi(\frac{1}{2}+18i)$ is therefore *negative*. Since $\xi(\frac{1}{2})$ is positive (ξ is positive on the entire real axis), it follows that *there is at least one root ρ on the line segment from $\frac{1}{2}$ to $\frac{1}{2}+18i$.* By computing further values of Z one could obtain more detailed information on the sign of $\xi(\frac{1}{2}+it)$ and therefore more precise information on the location of roots ρ on $\operatorname{Re} s=\frac{1}{2}$. However, the evaluation of Z requires *both* an evaluation of ζ *and* an evaluation of ϑ, and in order to locate roots ρ on $\operatorname{Re} s=\frac{1}{2}$, it suffices to evaluate just ζ—and in fact just $\operatorname{Im}\zeta$—provided one analyzes the result with a certain amount of ingenuity. Consider, for example, in Table IV the values of $\zeta(\frac{1}{2}+it)$ computed with two-place accuracy at intervals of 0.2 from $t=0$ to $t=50$.

Although these values were taken from Haselgrove's tables [H8], it would not be too lengthy to compute them from scratch using Euler–Maclaurin, particularly in view of the fact that there are economies of scale in computing many values of n^{it} ($n=2,3,4,\ldots$) which is the major operation in the Euler–Maclaurin evaluation of ζ. Now examination of this table leads to a few very elementary but very useful observations.

In the first place, the real part of ζ has a strong tendency to be positive. There are brief intervals, 11 in all, where $\operatorname{Re}\zeta$ is negative, but apart from the first one, which is clearly atypical, the longest of them is from 47.2 to 48.0

TABLE IV[a]

t	$\zeta(\frac{1}{2}+it)$	t	$\zeta(\frac{1}{2}+it)$	t	$\zeta(\frac{1}{2}+it)$
0.0	-1.46	9.0	$+1.45+0.19i$	18.0	$+2.33-0.19i$
0.2	$-1.18-0.67i$	9.2	$+1.48+0.14i$	18.2	$+2.27-0.43i$
0.4	$-0.68-0.94i$	9.4	$+1.51+0.08i$	18.4	$+2.17-0.66i$
0.6	$-0.28-0.94i$	9.6	$+1.53+0.02i$	18.6	$+2.02-0.86i$
0.8	$-0.02-0.84i$	9.8	$+1.54-0.04i$	18.8	$+1.84-1.03i$
1.0	$+0.14-0.72i$	10.0	$+1.54-0.12i$	19.0	$+1.62-1.16i$
1.2	$+0.25-0.62i$	10.2	$+1.54-0.19i$	19.2	$+1.38-1.24i$
1.4	$+0.32-0.52i$	10.4	$+1.53-0.26i$	19.4	$+1.13-1.28i$
1.6	$+0.37-0.44i$	10.6	$+1.50-0.34i$	19.6	$+0.88-1.26i$
1.8	$+0.41-0.37i$	10.8	$+1.47-0.42i$	19.8	$+0.65-1.18i$
2.0	$+0.44-0.31i$	11.0	$+1.42-0.49i$	20.0	$+0.43-1.06i$
2.2	$+0.46-0.26i$	11.2	$+1.36-0.56i$	20.2	$+0.25-0.90i$
2.4	$+0.48-0.21i$	11.4	$+1.29-0.62i$	20.4	$+0.11-0.70i$
2.6	$+0.50-0.16i$	11.6	$+1.21-0.67i$	20.6	$+0.02-0.48i$
2.8	$+0.52-0.12i$	11.8	$+1.12-0.71i$	20.8	$-0.02-0.25i$
3.0	$+0.53-0.08i$	12.0	$+1.02-0.75i$	21.0	$-0.01-0.02i$
3.2	$+0.55-0.04i$	12.2	$+0.91-0.76i$	21.2	$+0.06+0.19i$
3.4	$+0.56-0.01i$	12.4	$+0.79-0.76i$	21.4	$+0.18+0.38i$
3.6	$+0.58+0.03i$	12.6	$+0.68-0.75i$	21.6	$+0.34+0.52i$
3.8	$+0.59+0.06i$	12.8	$+0.56-0.71i$	21.8	$+0.52+0.62i$
4.0	$+0.61+0.09i$	13.0	$+0.44-0.66i$	22.0	$+0.72+0.67i$
4.2	$+0.62+0.12i$	13.2	$+0.33-0.58i$	22.2	$+0.92+0.66i$
4.4	$+0.64+0.15i$	13.4	$+0.23-0.49i$	22.4	$+1.11+0.60i$
4.6	$+0.66+0.18i$	13.6	$+0.15-0.38i$	22.6	$+1.26+0.49i$
4.8	$+0.68+0.21i$	13.8	$+0.07-0.25i$	22.8	$+1.38+0.34i$
5.0	$+0.70+0.23i$	14.0	$+0.02-0.10i$	23.0	$+1.45+0.16i$
5.2	$+0.73+0.26i$	14.2	$-0.01+0.05i$	23.2	$+1.46-0.03i$
5.4	$+0.75+0.28i$	14.4	$-0.01+0.21i$	23.4	$+1.41-0.21i$
5.6	$+0.78+0.30i$	14.6	$+0.01+0.38i$	23.6	$+1.30-0.38i$
5.8	$+0.81+0.32i$	14.8	$+0.07+0.55i$	23.8	$+1.14-0.50i$
6.0	$+0.84+0.34i$	15.0	$+0.15+0.70i$	24.0	$+0.95-0.58i$
6.2	$+0.87+0.36i$	15.2	$+0.26+0.85i$	24.2	$+0.73-0.60i$
6.4	$+0.91+0.37i$	15.4	$+0.39+0.98i$	24.4	$+0.51-0.55i$
6.6	$+0.94+0.38i$	15.6	$+0.56+1.09i$	24.6	$+0.30-0.43i$
6.8	$+0.98+0.39i$	15.8	$+0.74+1.17i$	24.8	$+0.13-0.25i$
7.0	$+1.02+0.40i$	16.0	$+0.94+1.22i$	25.0	$\pm 0.00-0.01i$
7.2	$+1.06+0.40i$	16.2	$+1.15+1.23i$	25.2	$-0.05+0.26i$
7.4	$+1.11+0.40i$	16.4	$+1.36+1.20i$	25.4	$-0.04+0.55i$
7.6	$+1.15+0.39i$	16.6	$+1.57+1.14i$	25.6	$+0.06+0.85i$
7.8	$+1.20+0.38i$	16.8	$+1.77+1.04i$	25.8	$+0.25+1.11i$
8.0	$+1.24+0.36i$	17.0	$+1.95+0.90i$	26.0	$+0.50+1.34i$
8.2	$+1.29+0.34i$	17.2	$+2.10+0.72i$	26.2	$+0.82+1.49i$
8.4	$+1.33+0.31i$	17.4	$+2.22+0.52i$	26.4	$+1.17+1.56i$
8.6	$+1.37+0.28i$	17.6	$+2.30+0.29i$	26.6	$+1.55+1.54i$
8.8	$+1.41+0.24i$	17.8	$+2.34+0.06i$	26.8	$+1.92+1.42i$

[a]Values from Haselgrove [H8].

TABLE IV *continued*[a]

t	$\zeta(\frac{1}{2}+it)$	t	$\zeta(\frac{1}{2}+it)$	t	$\zeta(\frac{1}{2}+it)$
27.0	$+2.25+1.21i$	35.0	$+2.60+1.11i$	43.0	$+0.44-0.31i$
27.2	$+2.53+0.91i$	35.2	$+2.84+0.67i$	43.2	$+0.16-0.16i$
27.4	$+2.73+0.55i$	35.4	$+2.94+0.17i$	43.4	$-0.07+0.11i$
27.6	$+2.83+0.15i$	35.6	$+2.89-0.33i$	43.6	$-0.20+0.50i$
27.8	$+2.83-0.27i$	35.8	$+2.70-0.80i$	43.8	$-0.18+0.94i$
28.0	$+2.72-0.68i$	36.0	$+2.38-1.19i$	44.0	$+0.01+1.40i$
28.2	$+2.52-1.05i$	36.2	$+1.97-1.46i$	44.2	$+0.37+1.80i$
28.4	$+2.23-1.35i$	36.4	$+1.50-1.59i$	44.4	$+0.87+2.08i$
28.6	$+1.87-1.57i$	36.6	$+1.03-1.57i$	44.6	$+1.47+2.19i$
28.8	$+1.48-1.69i$	36.8	$+0.60-1.40i$	44.8	$+2.11+2.10i$
29.0	$+1.09-1.70i$	37.0	$+0.26-1.12i$	45.0	$+2.71+1.80i$
29.2	$+0.71-1.61i$	37.2	$+0.04-0.76i$	45.2	$+3.21+1.31i$
29.4	$+0.38-1.43i$	37.4	$-0.05-0.36i$	45.4	$+3.54+0.69i$
29.6	$+0.13-1.18i$	37.6	$+0.01+0.03i$	45.6	$+3.66-0.03i$
29.8	$-0.04-0.89i$	37.8	$+0.19+0.36i$	45.8	$+3.56-0.74i$
30.0	$-0.12-0.58i$	38.0	$+0.46+0.59i$	46.0	$+3.24-1.39i$
30.2	$-0.11-0.29i$	38.2	$+0.80+0.71i$	46.2	$+2.75-1.90i$
30.4	$-0.02-0.03i$	38.4	$+1.14+0.69i$	46.4	$+2.14-2.22i$
30.6	$+0.14+0.17i$	38.6	$+1.44+0.55i$	46.6	$+1.49-2.33i$
30.8	$+0.33+0.30i$	38.8	$+1.67+0.31i$	46.8	$+0.86-2.24i$
31.0	$+0.52+0.34i$	39.0	$+1.79\pm 0.00i$	47.0	$+0.33-1.97i$
31.2	$+0.70+0.31i$	39.2	$+1.78-0.33i$	47.2	$-0.06-1.57i$
31.4	$+0.84+0.22i$	39.4	$+1.66-0.64i$	47.4	$-0.27-1.11i$
31.6	$+0.92+0.09i$	39.6	$+1.43-0.88i$	47.6	$-0.31-0.66i$
31.8	$+0.92-0.06i$	39.8	$+1.12-1.02i$	47.8	$-0.21-0.28i$
32.0	$+0.84-0.20i$	40.0	$+0.79-1.04i$	48.0	$-0.01-0.01i$
32.2	$+0.71-0.29i$	40.2	$+0.48-0.95i$	48.2	$+0.24+0.14i$
32.4	$+0.52-0.32i$	40.4	$+0.22-0.75i$	48.4	$+0.47+0.15i$
32.6	$+0.31-0.27i$	40.6	$+0.05-0.48i$	48.6	$+0.64+0.07i$
32.8	$+0.11-0.14i$	40.8	$-0.02-0.18i$	48.8	$+0.71-0.06i$
33.0	$-0.05+0.08i$	41.0	$+0.03+0.12i$	49.0	$+0.67-0.20i$
33.2	$-0.13+0.36i$	41.2	$+0.18+0.36i$	49.2	$+0.53-0.29i$
33.4	$-0.13+0.69i$	41.4	$+0.40+0.51i$	49.4	$+0.34-0.29i$
33.6	$-0.02+1.03i$	41.6	$+0.64+0.57i$	49.6	$+0.14-0.18i$
33.8	$+0.20+1.35i$	41.8	$+0.87+0.52i$	49.8	$-0.02+0.03i$
34.0	$+0.52+1.60i$	42.0	$+1.04+0.37i$	50.0	$-0.08+0.33i$
34.2	$+0.92+1.75i$	42.2	$+1.12+0.18i$		
34.4	$+1.37+1.79i$	42.4	$+1.08-0.04i$		
34.6	$+1.83+1.69i$	42.6	$+0.95-0.22i$		
34.8	$+2.25+1.46i$	42.8	$+0.72-0.32i$		

[a]Values from Haselgrove [H8].

and the value of Re ζ does not go much below -0.3 anywhere in the range $1 \leq t \leq 50$.

The sign of the imaginary part of ζ, on the other hand, oscillates fairly regularly between plus and minus. In fact, these oscillations are smooth enough and the passages through the value zero pronounced enough that one can be fairly certain that $\operatorname{Im} \zeta(\frac{1}{2} + it)$ has exactly 21 zeros in the range $0 < t \leq 50$, one in each of the 21 intervals where the table shows a sign change in Im ζ (between 3.4 and 3.6, between 9.6 and 9.8, etc.). Since $\xi(\frac{1}{2} + it) = 0$ if and only if $\operatorname{Re} \zeta(\frac{1}{2} + it) = 0$ *and* $\operatorname{Im} \zeta(\frac{1}{2} + it) = 0$, the problem of finding all roots ρ on the line segment from $\frac{1}{2}$ to $\frac{1}{2} + 50i$ is reduced to the problem of determining which, if any, of these 21 zeros of Im ζ are also zeros of Re ζ. Now 11 of them, namely, the first, second, fourth, sixth, eighth, . . . , eighteenth, and twentieth lie between points where Re ζ is strongly positive and clearly do not merit serious consideration as possible zeros. Judging from Table IV, however, it appears quite possible that any of the remaining 10—namely, the third, fifth, seventh, etc.—might be zeros of Re ζ. Now when $Z(t)$, $\vartheta(t)$ are defined as above, they are real-valued functions of the real variable t and

$$\begin{aligned}\zeta(\tfrac{1}{2} + it) &= e^{-i\vartheta(t)}Z(t)\\ &= Z(t)\cos\vartheta(t) - iZ(t)\sin\vartheta(t).\end{aligned}$$

Hence, $\operatorname{Im} \zeta(\frac{1}{2} + it) = -Z(t)\sin\vartheta(t)$ and a change of sign of Im ζ implies a change of sign of either $Z(t)$ or $\sin\vartheta(t)$. But even very rough calculations of $\vartheta(t)$ on the 10 intervals in question suffice to show that on these intervals $\vartheta(t)$ is nowhere near a multiple of π; therefore $\sin\vartheta(t)$ definitely does not change sign; therefore $Z(t)$ definitely does change sign; therefore there is definitely a zero of Z in the interval and a root ρ on the corresponding interval of Re $s = \frac{1}{2}$.

This proves the existence of 10 roots ρ on the line segment from $\frac{1}{2}$ to $\frac{1}{2} + 50i$ and locates them between $\frac{1}{2} + i14.0$ and $\frac{1}{2} + i14.2$, between $\frac{1}{2} + i21.0$ and $\frac{1}{2} + i21.2$, etc. To locate them more exactly, it suffices to estimate their position by linear interpolation (*regula falsi*) and calculate Im ζ more precisely. For example, linear interpolation suggests, since Im ζ goes from -0.10 to $+0.05$ as t goes from 14.0 to 14.2, that the zero lies two thirds of the way through the interval at 14.1333, and it is at this point that the value of Im ζ should be computed more exactly. This is precisely the method by which Gram computed the 15 roots given in Section 6.1.

The above calculations prove conclusively the existence of *at least* 10 roots ρ on the line segment from $\frac{1}{2}$ to $\frac{1}{2} + 50i$, and they strongly indicate—but do not prove—that there are no others on this line segment, but they give no information at all about possible roots *not* on the line Re $s = \frac{1}{2}$ in the range $0 \leq \operatorname{Im} s \leq 50$. However, Gram did prove, as will be explained in the next section, that the 10 roots he had found are the *only* roots in the range $0 \leq \operatorname{Im} s \leq 50$, and therefore that the Riemann hypothesis is true in this range.

Consider now the problem of locating more roots beyond $t = 50$. Since the computation of $\zeta(\frac{1}{2} + it)$ becomes increasingly long as t increases, it is desirable to use as few evaluations of $\zeta(\frac{1}{2} + it)$ as possible. Now in the range $10 \leq t \leq 50$ the zeros of $\operatorname{Im} \zeta$ follow a very simple pattern, namely, *in this range the zeros of* $\operatorname{Im} \zeta = Z \sin \vartheta$ *are alternately zeros of* Z *and zeros of* $\sin \vartheta$. Gram showed that it is not unlikely that this pattern persists, at least for a while, past $t = 50$ and he also showed that the zeros of $\sin \vartheta$ are quite easy to find. These two observations simplify considerably the search for further zeros.

Gram gave the following reasons for believing that the alternation of zeros of Z with zeros of $\sin \vartheta$ will persist beyond $t = 50$. In the first place, this phenomenon is closely related to the fact that $\operatorname{Re} \zeta$ has a strong tendency to be positive. To see this relation note first that the approximation

$$\frac{d}{ds} \log \Pi(s) \sim \log s$$

[see (4) of Section 6.3] shows that the derivative of $\vartheta(t)$ is

$$\operatorname{Im} \frac{i}{2} \frac{\Pi'\left(\frac{it}{2} - \frac{3}{4}\right)}{\Pi\left(\frac{it}{2} - \frac{3}{4}\right)} - \frac{1}{2} \log \pi \sim \frac{1}{2} \log \left| \frac{it}{2} - \frac{3}{4} \right| - \frac{1}{2} \log \pi$$
$$\sim \frac{1}{2} \log \frac{t}{2\pi}$$

from which it can easily be shown that $\vartheta'(t) > 0$ for $t \geq 10$. Thus ϑ is an increasing function of t, between consecutive zeros of $\sin \vartheta$ there is exactly one zero of $\cos \vartheta$, and $\cos \vartheta$ changes sign. Therefore if $\operatorname{Re} \zeta = Z \cos \vartheta$ is positive at two consecutive zeros of $\sin \vartheta$—which is likely in view of the preponderance of positive values of $\operatorname{Re} \zeta$—it follows that Z changes sign and hence that there is at least one zero of Z between these two consecutive zeros of $\sin \vartheta$. Since the first failure, if there is one, in the pattern of alternation would naturally be expected to be a pair of consecutive zeros of $\sin \vartheta$ between which there would be either 2 or 0 zeros of Z, the first failure, if there is one, should be indicated by a zero of $\sin \vartheta$, where $\operatorname{Re} \zeta$ is negative instead of positive. The zeros of $\sin \vartheta$ are called *Gram points*, and the conclusion is that the persistence of the pattern of alternation of zeros of Z with Gram points is closely related to the persistence of the positivity of $\operatorname{Re} \zeta$ at Gram points. But Gram argued that the predominance of positive values of $\operatorname{Re} \zeta$ is due to the fact that the Euler–Maclaurin formula for $\zeta(\frac{1}{2} + it)$ *begins* with a $+1$ in the real part and to the fact that, as long as it is not necessary to use too large a value of N, it will be unusual for the smaller† terms which follow to combine to over-

†The negative values of $\operatorname{Re} \zeta$ which occur for small values of t result, as is seen immediately from the computation of $\zeta(\frac{1}{2})$ in the preceding section, from the fact that the term $N^{1-s}/(s - 1)$ then has a large negative real part. This term becomes small as t increases.