CHAPTER 3

SUMMATION

3.1. Introduction

We shall consider sums of the type $\sum_{k=1}^{n} a_k(n)$, where both the terms and the number of terms depend on n. We ask for asymptotic information about the value of the sum for large values of n. In many applications, $a_k(n)$ is independent of n, and actually several of our examples will be of this type, but the methods by which those examples are tackled, are by no means restricted to this case.

It is of course difficult to say anything in general. The asymptotic problem can be difficult, especially in cases where the a_k are not all of one sign, and where $\sum_1^n a_k(n)$ can be much smaller than $\sum_1^n |a_k(n)|$. On the other hand, there is a class of routine problems arising in many parts of analysis, and to which a large part of this chapter is devoted: the cases where all $a_k(n)$ are of one sign and where moreover the $a_k(n)$ "behave smoothly". We shall not attempt to define what smoothness of behaviour is, but we merely give a number of examples. These fall under four headings *a*, *b*, *c*, *d*, according to the location of the terms which give the main contribution to the sum. The major contribution can come from:

a. a comparatively small number of terms at the end, or at the beginning.

b. a single term at the end or at the beginning.

c. a comparatively small number of terms somewhere in the middle.

There is also a case *d*, where there is not such a small group of terms whose sum dominates the sum of all others.

3.2. Case a

Our first example concerns the behaviour of the sum $s_n = \sum_{k=1}^{n} k^{-3}$. A first approximation to s_n is the sum $S = \sum_1^\infty k^{-3}$ of

the infinite series, and the error term is $-\sum_{n+1}^{\infty} k^{-3}$. For this last sum we easily obtain the estimate $O(n^{-2})$, e.g. by

$$\sum_{n+1}^{\infty} k^{-3} < \sum_{n+1}^{\infty} \int_{k-1}^{k} t^{-3}dt = \int_{n}^{\infty} t^{-3}dt = \tfrac{1}{2}n^{-2}, \tag{3.2.1}$$

and therefore

$$s_n = S + O(n^{-2}) \qquad (n \to \infty). \tag{3.2.2}$$

Results of this type are quite satisfactory for many analytical purposes; it should be noted, however, that from the point of view of numerical analysis nothing has been achieved by (3.2.2), unless we know the value of S from other sources of information. The numerical analyst would prefer to evaluate $\sum_1^m k^{-3}$ for some suitably chosen value of m, and to estimate $\sum_{m+1}^{n} k^{-3}$.

Formula (3.2.2) can be improved by refinement of the argument used in (3.2.1), i.e. comparison of the sum with the integral. We shall return to this technique in secs. 3.5 and 3.6.

Our next example is $\sum_1^n 2^k \log k$. In this sum there is a relatively small number of terms at the end whose total contribution is large compared to the sum of all others. If we omit the last $[\log n]$ terms ($[\log n]$ denotes the largest integer $\leq \log n$), the sum of the remaining terms is less than

$$\sum_{1}^{n-[\log n]} 2^k \log n \leq 2^{n+1-\log n} \log n = 2^{n+1} n^{-\log 2} \log n,$$

and this is much smaller than the n-th term.

We notice that $\log k$ shows but little variation when k runs through the indices of the $[\log n]$ significant terms. We therefore expand $\log k$ in terms of powers of $(n-k)/n$, and in doing this we can easily admit the range $\tfrac{1}{2}n < k \leq n$. We shall be satisfied with

$$\log k = \log(n-h) = \log n - hn^{-1} + O(h^2n^{-2}) \quad (n \to \infty)$$

which holds uniformly in h $(0 \leqslant h < \tfrac{1}{2}n)$. We now evaluate

$$\sum_{1 \leq k \leq \frac{1}{2}n} 2^k \log k = O(2^{\frac{1}{2}n} \log n),$$

$$\sum_{\frac{1}{2}n < k \leq n} 2^k \log n = 2^{n+1} \log n + O(2^{\frac{1}{2}n} \log n),$$

$$\sum_{\frac{1}{2}n < k \leq n} 2^k hn^{-1} = n^{-1}2^n \sum_{h=1}^{\infty} 2^{-h}h + O(2^{\frac{1}{2}n}),$$

$$\sum_{\frac{1}{2}n < k \leq n} 2^k O(h^2n^{-2}) = O(2^n n^{-2}) \cdot \sum_{h=1}^{\infty} 2^{-h}h^2.$$

The main error term is $O(2^n n^{-2})$; the terms involving $2^{\frac{1}{2}n}$ are much smaller than this one. Our result is

$$2^{-n}\sum_{1}^{n} 2^k \log k = 2\log n - n^{-1}\sum_{1}^{\infty} h\cdot 2^{-h} + O(n^{-2}),$$

and it is not difficult to extend our argument in order to obtain an asymptotic series in terms of powers of n^{-1}:

$$2^{-n}\sum_{k=1}^{n} 2^k \log k - 2\log n \approx c_1 n^{-1} + c_2 n^{-2} + \dots \qquad (n\to\infty),$$

with $c_j = -j^{-1}\sum_{h=1}^{\infty} h^j 2^{-h}$.

3.3. Case b

We are often confronted with sums of positive terms, where each term has at least the order of magnitude of the sum of all previous terms. Our example is $s_n = \sum_{k=1}^{n} k!$. Dividing by the last term, we find that

$$\frac{s_n}{n!} = 1 + \frac{1}{n} + \frac{1}{n(n-1)} + \frac{1}{n(n-1)(n-2)} + \dots + \frac{1}{n!}.$$

If we stop after the 5th term, say, we neglect $n-5$ terms, each one of which is at most $(n-5)!/n!$, and so the error is $O(n^{-4})$. But the 5th term itself is $O(n^{-4})$, and therefore

$$\frac{s_n}{n!} = 1 + \frac{1}{n} + \frac{1}{n(n-1)} + \frac{1}{n(n-1)(n-2)} + O(n^{-4}) \qquad (n\to\infty).$$

If we so wish, we can expand these terms into powers of n^{-1}:

$$\frac{s_n}{n!} = 1 + \frac{1}{n} + \frac{1}{n^2} + \frac{2}{n^3} + O(n^{-4}) \qquad (n\to\infty).$$

Replacing the number 5 by an arbitrary integer, we easily find that there is an asymptotic expansion

(3.3.1) $\quad s_n/n! \approx c_0 + c_1 n^{-1} + c_2 n^{-2} + \dots \qquad (n\to\infty).$

This series is not convergent, that is to say, the series $c_0 + c_1 x + c_2 x^2 + \dots$ does not converge unless $x = 0$.

This can be shown as follows. The series $c_0 + c_1 x + c_2 x^2 + \dots$ arises as the formal sum of the power series for the functions

$$1,\ x,\ \frac{x^2}{1-x},\ \frac{x^3}{(1-x)(1-2x)},\ \frac{x^4}{(1-x)(1-2x)(1-3x)},\ \dots,$$

and each one of these has non-negative coefficients. So if k is any positive integer, the coefficients of $c_0 + c_1 x + c_2 x^2 + \dots$ exceed those of the series for $x^{k+1}/(1-x)(1-2x)\cdots(1-kx)$. The latter series diverges at $x = k^{-1}$, and therefore $c_0 + c_1 x + c_2 x^2 + \dots$ diverges at $x = k^{-1}$. Since k is arbitrary, we infer that the radius of convergence of $c_0 + c_1 x + c_2 x^2 + \dots$ is zero.

There is usually no reason to try to obtain an explicit formula for the coefficients of a divergent asymptotic series. For practical purposes only a few terms of the asymptotic series will be needed, and for nearly all theoretical purposes the mere existence of an asymptotic series is already a satisfactory result. So it is only for the sake of curiosity that we mention that $c_{k+1} = k!d_k$ ($k = 0, 1, 2, \dots$), where the d_k are the coefficients in

$$\exp(e^x - 1) = \sum_{0}^{\infty} d_k x^k.$$

We leave the proof to the reader [Hint: first prove, e.g. by induction, that

$$\int_0^\infty e^{-y/x}\frac{(e^y-1)^k}{k!}\,dy = \frac{x^{k+1}}{(1-x)(1-2x)\cdots(1-kx)} \qquad (0 < x < k^{-1});$$

then notice that the coefficient of x^{j+1} on the left equals $j!$ times the coefficient of y^j in $(e^y-1)^k/k!$].

3.4. Case c

A typical example is

$$s_n = \sum_{k=1}^{n} a_k(n), \quad a_k(n) = 2^{2k}\{n!/k!(n-k)!\}^2.$$

We have $a_{k+1}(n)/a_k(n) = \{2(n-k)/(k+1)\}^2$. Hence the maximal term occurs at the first value of k for which $2(n-k) < (k+1)$, that is, at about $k = 2n/3$.

We notice that in this case, contrary to our previous examples, the sum is large compared to the value of the maximal term. For, if we move k in either direction, starting from the maximal term, then $a_k(n)$ decreases rather slowly (n is considered to be fixed). It can be shown by various methods, e.g. by the Stirling formula for the factorials, that the number of terms which exceed $\frac{1}{2}\max a_k(n)$, is of the order of $n^{\frac{1}{2}}$. If, however, $|k - 2n/3|$ is much greater than $n^{\frac{1}{2}}$, then a_k is very small compared to the maximum, and also the total contribution of these terms is relatively small. Therefore we have to focus our attention on regions of the type $|k - 2n/3| < An^{\frac{1}{2}}$.

By application of the Stirling formula, $a_k(n)$ can be succesfully approximated in this region, and then sums are obtained resembling the one discussed in sec. 3.9. We leave it at these brief remarks.

3.5. Case d

As a first example we take $a_k = k^{\frac{1}{2}}$. The ideal technique for dealing with a case as smooth as this one is given by the Euler-Maclaurin sum formula. Nevertheless we shall start with a more elementary method, which can be applied in less regular cases as well.

There are two steps. First approximate a_k by a sequence u_k which is such that $\sum_{k=1}^n u_k$ is explicitly known; the approximation has to be strong enough for $\sum_{k=1}^\infty (a_k - u_k)$ to converge. The second step deals with $\sum_{k=1}^n (a_k - u_k)$. The first approximation to this sum is, as in sec. 3.2, the infinite sum $S = \sum_{k=1}^\infty (a_k - u_k)$, and we have

$$(3.5.1) \qquad s_n = \sum_{k=1}^n a_k = \sum_{k=1}^n u_k + S + \sum_{k=n+1}^\infty (u_k - a_k).$$

In the last sum we try to approximate $u_k - a_k$ by a sequence v_k, such that $\sum_{n+1}^\infty v_k$ is explicitly known, and such that the error term $\sum_{n+1}^\infty (u_k - a_k - v_k)$ is known to be small. This procedure can be continued.

The weak point in the procedure is that in general there is hardly any information about the value of S. The situation is not as serious as in (3.2.2), for in (3.5.1) the major contribution is not S, but the sum $\sum_1^n u_k$, whose value is known.

In our example $a_k = k^{\frac{1}{2}}$ we can obtain a first approximation to the sum s_n by taking the integral $\int_0^n t^{\frac{1}{2}} dt = \frac{2}{3} n^{3/2}$. If we now try to take u_k such that $\sum_1^n u_k = \frac{2}{3} n^{3/2}$, we still fail. For

$$(3.5.2) \qquad k^{\frac{1}{2}} - \{\tfrac{2}{3} k^{3/2} - \tfrac{2}{3}(k-1)^{3/2}\}$$

is not yet the k-th term of a convergent series. On expanding $(1 - k^{-1})^{3/2}$ into powers of k^{-1} by the binomial series, we find that the expression (3.5.2) is $\frac{1}{4}k^{-\frac{1}{2}} + O(k^{-3/2})$, and $\sum k^{-\frac{1}{2}}$ diverges. But we can again approximate the partial sums of $\sum k^{-\frac{1}{2}}$ by an integral, viz. $2n^{\frac{1}{2}}$. If we now take new u_k's, viz.

$$u_k = U_k - U_{k-1}, \qquad U_k = \tfrac{2}{3}k^{3/2} + \tfrac{1}{2}k^{\frac{1}{2}},$$

we easily obtain that

$$(3.5.3) \qquad u_k - a_k = k^{-3/2}/48 + O(k^{-5/2}) \qquad (k \to \infty),$$

whence $\sum_{k=1}^\infty (u_k - a_k)$ converges.

In the second step we have to approximate $u_k - a_k$ by a sequence v_k. We take $v_k = V_{k-1} - V_k$, where

$$V_k = k^{-\frac{1}{2}}/24, \quad \sum_{n+1}^\infty v_k = V_n,$$

as suggested by the integral

$$\int_n^\infty (t^{-3/2}/48)dt = n^{-\frac{1}{2}}/24.$$

We so obtain

$$u_k - a_k - v_k = O(k^{-5/2}),$$

and, by (3.5.1),

$$(3.5.4) \qquad \sum_{k=1}^n k^{\frac{1}{2}} = \tfrac{2}{3}n^{3/2} + \tfrac{1}{2}n^{\frac{1}{2}} + S + \tfrac{1}{24}n^{-\frac{1}{2}} + O(n^{-3/2}) \quad (n \to \infty).$$

The term $O(n^{-3/2})$ can be replaced by an asymptotic series, for the process can be carried on and we can get as many terms as we please. To this end it is, of course, necessary to refine (3.5.3). This is easily done, for $(u_k - a_k)k^{3/2}$ can be expanded into powers of k^{-1}, and the expansion converges if $k > 1$.

We next ask for the value of S. We obviously have

$$(3.5.5) \quad S = \sum_{k=1}^\infty \{k^{\frac{1}{2}} - \tfrac{2}{3}k^{3/2} - \tfrac{1}{2}k^{\frac{1}{2}} + \tfrac{2}{3}(k-1)^{3/2} + \tfrac{1}{2}(k-1)^{\frac{1}{2}}\} = \lim_{n\to\infty} \{\sum_{k=1}^n k^{\frac{1}{2}} - U_n\},$$

but it is possible to derive a simpler expression.

The method depends on analyticity properties, and therefore it is not generally applicable.

We first generalize (3.5.4) by introducing a complex parameter z.

Instead of (3.5.4) we obtain, by the same method,

$$\sum_{k=1}^{n} k^{-z} = \frac{n^{1-z}}{1-z} + \tfrac{1}{2}n^{-z} + S(z) + O(n^{-z-1}) \qquad (n \to \infty), \tag{3.5.6}$$

if $\operatorname{Re} z > -1$, $z \neq 1$. Here $S(z)$ is the sum of a convergent series, analogous to (3.5.5). Furthermore, it is not hard to show that this sum is an analytic function of z in the region $\operatorname{Re} z > -1$, $z \neq 1$. If $\operatorname{Re} z > 1$, it represents the Riemann zeta function [1] $\zeta(z) = \sum_1^\infty n^{-z}$, as can be seen from (3.5.6) by making $n \to \infty$. Therefore $S(z) = \zeta(z)$ in the whole region.

Especially, the value of (3.5.5) is

$$S(-\tfrac{1}{2}) = \zeta(-\tfrac{1}{2}) = -\zeta(\tfrac{3}{2})/4\pi.$$

The latter equality follows from the functional equation $\zeta(1-s) = 2^{1-s}\pi^{-s}\Gamma(s) \cos \tfrac{1}{2}\pi s\, \zeta(s)$.

3.6. The Euler-Maclaurin sum formula

Our considerations of sec. 3.5 were meant to demonstrate a method, rather than giving the shortest way to deal with $\sum_1^n k^{\frac{1}{2}}$. It seems that the shortest and most efficient way of dealing with such cases depends on the Euler-Maclaurin sum formula. It is incorporated in many textbooks of advanced analysis [2], and therefore we omit its proof.

The basic formula is

$$\left\{\begin{aligned} &\frac{g(0)+g(1)}{2} - \int_0^1 g(x)dx = \\ &\quad = \{g'(1) - g'(0)\}\frac{B_2}{2!} + \{g'''(1) - g'''(0)\}\frac{B_4}{4!} + \dots + \\ &\quad + \{g^{(2m-1)}(1) - g^{(2m-1)}(0)\}\frac{B_{2m}}{(2m)!} - \int_0^1 g^{(2m)}(x)\frac{B_{2m}(x)}{(2m)!}dx. \end{aligned}\right. \tag{3.6.1}$$

Here m represents any integer ≥ 1, and g is a function having $2m$ continuous derivatives in the interval $0 \leq x \leq 1$. The B's are the Bernoulli numbers, defined by

$$z/(e^z - 1) = \sum_0^\infty B_n z^n/n! \qquad (|z| < 2\pi),$$

whence

$$\begin{aligned} &B_0 = 1, B_1 = -\tfrac{1}{2}, B_2 = \tfrac{1}{6}, B_3 = B_5 = B_7 = \dots = 0, \\ &B_4 = -\tfrac{1}{30}, B_6 = \tfrac{1}{42}, B_8 = -\tfrac{1}{30}, B_{10} = \tfrac{5}{66}, \\ &B_{12} = -\tfrac{691}{2730}, B_{14} = \tfrac{7}{6}, B_{16} = -\tfrac{3617}{510}, \dots . \end{aligned}$$

Finally, the $B_n(t)$ denote the Bernoulli polynomials, defined by

$$ze^{zt}/(e^z - 1) = \sum_0^\infty B_n(t) z^n/n!.$$

If we write down (3.6.1) for the functions $g(x) = f(x+1)$, $g(x) = f(x+2)$, $\dots$, $g(x) = f(x+n-1)$, respectively, and if we add the results, many terms cancel out, and we get the Euler-Maclaurin sum formula. We write it in the form

$$\left\{\begin{aligned} &f(1) + \dots + f(n) = \int_1^n f(x)dx + C + \tfrac{1}{2}f(n) + \\ &\quad + \frac{B_2}{2!}f'(n) + \frac{B_4}{4!}f'''(n) + \dots + \\ &+ \frac{B_{2m}}{(2m)!}f^{(2m-1)}(n) - \int_1^n f^{(2m)}(x)\frac{B_{2m}(x-[x])}{(2m)!}dx. \end{aligned}\right. \tag{3.6.2}$$

The function f is assumed to have $2m$ continuous derivatives if $x \geq 1$. The symbol $[x]$ has the usual meaning of the largest integer $\leq x$. $B_{2m}(x-[x])$ is the value of the $2m$-th Bernoulli polynomial at $x - [x]$. The number C is independent of n:

$$C = \tfrac{1}{2}f(1) - B_2 f'(1)/2! - \dots - B_{2m} f^{(2m-1)}(1)/(2m)!.$$

It is known that [1]

$$B_{2m}(x-[x]) = 2(2m)!(2\pi)^{-2m}(-1)^{m+1}\sum_{k=1}^\infty k^{-2m}\cos(2k\pi x)$$

if $m = 1, 2, 3, \dots$, whence it follows that

$$|B_{2m}(x-[x])| \leq |B_{2m}| = 2(2m)!\,(2\pi)^{-2m}\sum_{k=1}^\infty k^{-2m}.$$

[1] See E. T. Whittaker and G. N. Watson, Modern Analysis, 4th ed., Cambridge 1946, ch. 13.

[2] Ibid., § 7.21. Our notation for the Bernoulli numbers and polynomials is slightly different, however.

[1] See W. Rogosinski, Fourier Series, Chelsea, New York, ch. 2, § 4.

This gives a satisfactory estimate for the remainder term in (3.6.1).

If $f(x)$ is such that $\int_0^\infty |f^{(2m)}(x)|dx$ converges, we immediately have an asymptotic formula:

$$(3.6.3)\qquad f(1) + \ldots + f(n) = \int_1^n f(x)dx + S + \tfrac{1}{2}f(n) +$$
$$+ \sum_{k=1}^{m} B_{2k} f^{(2k-1)}(n)/(2k)! + O\Big(\int_n^\infty |f^{(2m)}(x)|dx\Big) \qquad (n \to \infty),$$

where m is a fixed positive integer, and

$$S = C - \int_1^\infty f^{(2m)}(x)\,\frac{B_{2m}(x-[x])}{(2m)!}\,dx.$$

3.7. Example

Let z be a complex number, and $f(x) = x^{-z}\log x$. Then (3.6.3) can be applied if $2m > 1 - \operatorname{Re} z$. It results that

$$\sum_{k=1}^{n} k^{-z}\log k = \int_1^n x^{-z}\log x\,dx + C(z) + \tfrac{1}{2}n^{-z}\log n + R(n;z),$$

where $C(z)$ depends on z only, and $R(n;z)$ has an asymptotic expansion

$$R(n;z) \approx \frac{B_2}{2!}(n^{-z}\log n)' + \frac{B_4}{4!}(n^{-z}\log n)''' + \ldots \qquad (n\to\infty).$$

The accents denote differentiation with respect to n, evaluated as if n were a continuous variable.

As in sec. 3.5, $C(z)$ can be determined by an analyticity argument; we obtain $C(z) = -(1-z)^{-2} - \zeta'(z)$. The special case $z = 0$ gives the Stirling formula for $\log n!$, as [1] $\zeta'(0) = -\tfrac{1}{2}\log 2\pi$. It should be remarked, however, that there are many other methods for determining the value of $C(0)$ (see sec. 3.10).

3.8. A remark

Roughly speaking, the Euler-Maclaurin method does not work if the largest term, $f(n)$, say, is *not* small compared to the sum $f(1) + \ldots + f(n)$. In that case one cannot expect the order of $f^{(2m)}(n)$ to be lower than the one of $f(n)$, and so the Euler-Maclaurin formula does not give anything better than $f(1) + \ldots + f(n) = O(f(n))$. One can illustrate this by the example $\sum_1^n k!$ of sec. 3.3.

[1]) See E. T. WHITTAKER and G. N. WATSON, Modern Analysis, 4th ed., Cambridge 1946, § 13.21.

3.9. Another example

The Euler-Maclaurin method can also be applied to sums $\sum_{k=1}^n a_k(n)$ where the terms depend both on k and n. There is, however, no point in passing from (3.6.2) to (3.6.3) in that case, for then S will depend on n. An unspecified constant may often be tolerated in an asymptotic formula, but having an unspecified function of n just means having no formula at all. There are some cases, however, where

$$\int_1^n f^{(2m)}(x)B_{2m}(x-[x])/(2m)!\,dx$$

raises no difficulties, e.g. when $\int_1^n |f^{(2m)}(x)|dx$ is relatively small.

As an example we take

$$s_n = \sum_{k=-n}^{n} e^{-k^2\alpha/n},$$

where α is a positive constant. The Euler-Maclaurin formula gives, if $f(x) = e^{-x^2\alpha/n}$,

$$(3.9.1)\quad s_n = \int_{-n}^{n} f(x)dx + \tfrac{1}{2}f(n) + \tfrac{1}{2}f(-n) + B_2\{f'(n) - f'(-n)\}/2! +$$
$$+ \ldots + B_{2m}\{f^{(2m-1)}(n) - f^{(2m-1)}(-n)\}/(2m)! + R_n,$$

where

$$(3.9.2)\qquad R_m = -\int_{-n}^{n} f^{(2m)}(x)\,\frac{B_{2m}(x-[x])}{(2m)!}\,dx,$$

whence

$$|R_m| \le \frac{|B_{2m}|}{(2m)!}\int_{-n}^{n} |f^{(2m)}(x)|dx.$$

We have

$$\int_{-n}^{n} f(x)dx = \int_{-\infty}^{\infty} f(x)dx + \varepsilon_n = (\pi n/\alpha)^{\frac{1}{2}} + \varepsilon_n,$$

where the error term ε_n is $O(e^{-bn})$ with some positive constant b. Such errors are called *exponentially small*.

The other terms of (3.9.1), apart from R_n, are all exponentially small because of the fact that every derivative of $f(x)$ is of the type $P(x)f(x)$, where $P(x)$ is a polynomial. So everything depends on how well R_m can be estimated.

On substituting $x = y(n/2\alpha)^{\frac{1}{2}}$ we obtain

$$(3.9.3) \qquad \int_{-\infty}^{\infty} |f^{(2m)}(x)|dx = (2\alpha/n)^{m-\frac{1}{2}} \int_{-\infty}^{\infty} |(d/dy)^{2m} e^{-\frac{1}{2}y^2}|dy,$$

and it follows that $|R_m| < C_m n^{\frac{1}{2}-m}$, where C_m is positive and independent of n. Hence we have, for every m,

$$(3.9.4) \qquad s_n = (\pi n/\alpha)^{\frac{1}{2}} + O(n^{\frac{1}{2}-m}) \quad (n \to \infty).$$

In the case of s_n we accidentally have direct information from another source, viz. a theta function transformation formula, which gives a very good estimate. It is therefore interesting to compare this one to the result of the Euler-Maclaurin method.

For convenience we discuss the infinite sum instead of the finite one. (The difference between the two is exponentially small). Writing down the analogue of (3.9.1) for $\sum_{-N}^{N} e^{-k^2\alpha/n}$, and making $N \to \infty$, we obtain

$$(3.9.5) \qquad S_n = \sum_{k=-\infty}^{\infty} e^{-k^2\alpha/n} =$$
$$= (\pi n/\alpha)^{\frac{1}{2}} - \int_{-\infty}^{\infty} f^{(2m)}(x) B_{2m}(x-[x])/(2m)!\, dx,$$

where again $f(x) = e^{-x^2\alpha/n}$.

We denote the integral by R^*; it follows from (3.9.5) than R^* does not depend on m. What we shall call here the Euler-Maclaurin method consists of estimating

$$(3.9.6) \qquad |R^*| \leq \frac{|B_{2m}|}{(2m)!} \int_{-\infty}^{\infty} |f^{(2m)}(x)|dx$$

and choosing m such that the right-hand-side is minimal.

The theta transformation formula gives [1])

$$\sum_{k=-\infty}^{\infty} e^{-k^2\alpha/n} = (\pi n/\alpha)^{\frac{1}{2}} \sum_{k=-\infty}^{\infty} e^{-k^2\pi^2 n/\alpha},$$

and therefore

$$(3.9.7) \qquad -R^* = 2(\pi n/\alpha)^{\frac{1}{2}} e^{-\pi^2 n/\alpha} + O(n^{\frac{1}{2}} e^{-4\pi^2 n/\alpha}) \quad (n \to \infty).$$

We shall now investigate whether (3.9.6) can give anything as strong as this. It gives immediately that, for every m, we have $R^* = O(n^{\frac{1}{2}-m})$. For m fixed, this is very much weaker than (3.9.7), but by deriving uniform estimates and by taking m to be a suitable function of n, we can obtain a better result. There is of course no hope of proving (3.9.7), but it is interesting to see that the Euler-Maclaurin method can still show that $R^* = O(ne^{-\pi^2 n/\alpha})$, restricting the losses to the factor $n^{\frac{1}{2}}$.

If we adopt the definition

$$H_k(y) = (-1)^k e^{\frac{1}{2}y^2} (d/dy)^k e^{-\frac{1}{2}y^2}$$

for the Hermite polynomials, the integrand on the right-hand-side of (3.9.3) equals $e^{-\frac{1}{2}y^2}|H_{2m}(y)|$.

Using the integral representation

$$H_{2m}(y) = (2\pi)^{-\frac{1}{2}} e^{\frac{1}{2}y^2} \left(\frac{d}{dy}\right)^{2m} \int_{-\infty}^{\infty} e^{-\frac{1}{2}v^2+ivy}\, dv =$$
$$= (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} (iv)^{2m} e^{-\frac{1}{2}v^2+ivy+\frac{1}{2}y^2} dv = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} (y-iu)^{2m} e^{-\frac{1}{2}u^2}\, du,$$

we infer that

$$\int_{-\infty}^{\infty} |f^{(2m)}(x)|dx \leq (2\alpha/n)^{m-\frac{1}{2}} (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-\frac{1}{2}(y^2+u^2)} (y^2+u^2)^m du dy.$$

Introducing polar coordinates in the u-y-plane we easily find that the repeated integral equals $2^{m+1}\pi m!$.

The factor $|B_{2m}|/(2m)!$ occurring in (3.9.6) is equal to $2(2\pi)^{-2m}\zeta(2m)$ (see sec. 3.6), and therefore it is less than $C(2\pi)^{-2m}$,

---

[1]) See E. T. Whittaker and G. N. Watson, Modern Analysis, 4th ed., Cambridge 1946, § 21.51.

A simple direct proof is obtained by taking $f(x) = \exp(-\beta x^2)$, $a = 0$ $(\beta = \alpha/n)$ in Poisson's formula (3.12.1).

where C is an absolute constant. It now follows from (3.9.6) that

$$|R^*| < C(2\pi)^{-2m}(2\alpha/n)^{m-\frac{1}{2}}(2\pi)^{-\frac{1}{2}}2^{m+1}\pi m!.$$

Using Stirling's formula for $m!$ we infer that there is an absolute constant C_1 such that for all m and n

$$|R^*| < C_1(\alpha m/\pi^2 ne)^m(nm/2\alpha)^{\frac{1}{2}}. \tag{3.9.8}$$

It is now the right moment to fix the value of m. The minimum of $(\alpha t/\pi^2 ne)^t$ is easily seen to be attained at $t = \pi^2 n/\alpha$, and the value is $e^{-\pi^2 n/\alpha}$. However, m has to be an integer, and so we shall take $m = m_0 = [\pi^2 n/\alpha]$. In order to analyse the difference it makes, we put

$$\psi(\rho) = \rho \log(\alpha\rho/\pi^2 e)$$

whose minimum is $-\pi^2/\alpha$, attained at $\rho = \rho_0 = \pi^2/\alpha$. We have $\psi'(\rho_0) = 0$, and hence

$$\psi(m_0/n) = \psi\{\rho_0 + O(n^{-1})\} = -\pi^2/\alpha + O(n^{-2}).$$

If we now choose $m = m_0$, (3.9.8) becomes

$$R^* = O(ne^{-\pi^2 n/\alpha}) \qquad (n \to \infty).$$

3.10. The Stirling formula for the Γ-function in the complex plane

In the following, the Euler-Maclaurin formula will play about the same rôle as it did in (3.9.5). We shall have a sum containing a parameter z. For a fixed value of z we shall increase the number of terms indefinitely, and only afterwards we allow $|z|$ to tend to infinity (in (3.9.5) that parameter was n).

Let z be a real or complex number, not lying on the negative part of the real axis, and not equal to zero. We shall apply the Euler-Maclaurin formula to the sum

$$S_n(z) = \sum_{k=1}^{n} \log(z + k - 1),$$

where the logarithms are given their principal values (imaginary parts of the logarithms absolutely less than π). With an arbitrary integer $m \geq 1$ we obtain

$$S_n(z) = \tfrac{1}{2}\log z + \tfrac{1}{2}\log(z + n - 1) + \int_1^n \log(z + x - 1)dx + \\ + \sum_{k=1}^{m} \{(z + n - 1)^{1-2k} - z^{1-2k}\}(2k)^{-1}(2k - 1)^{-1}B_{2k} + \\ + \int_1^n (z + x - 1)^{-2m}(2m)^{-1}B_{2m}(x - [x])dx.$$

With z fixed we easily get an asymptotic formula with an error term $o(1)$:

$$S_n(z) = (z - \tfrac{1}{2})\log n - (z - \tfrac{1}{2})\log z + n\log n + \\ + z - n - \rho(z) + o(1) \qquad (n \to \infty), \tag{3.10.1}$$

where

$$\rho(z) = \sum_{k=1}^{m} z^{1-2k}(2k)^{-1}(2k - 1)^{-1}B_{2k} - \\ - \int_0^\infty (z + x)^{-2m}(2m)^{-1}B_{2m}(x - [x])dx. \tag{3.10.2}$$

As $\rho(z)$ does not depend on n, it is obvious from (3.10.1) that it does not depend on m either. This fact can also be shown from (3.10.2), integrating by parts.

Taking the difference $S_n(z) - S_n(1)$, we obtain, applying (3.10.1) twice,

$$S_n(z) - S_n(1) = (z-1)\log n - (z - \tfrac{1}{2})\log z + z - 1 + \\ + \rho(1) - \rho(z) + o(1) \qquad (n \to \infty). \tag{3.10.3}$$

This difference is connected with Euler's product formula for $\Gamma(z)$:

$$\Gamma(z) = \lim_{n\to\infty} n^{z-1}n!/z(z + 1)(z + 2)\cdots(z + n - 1). \tag{3.10.4}$$

Taking logarithms, we find:

$$\log \Gamma(z) = \lim_{n\to\infty}\{(z - 1)\log n + S_n(1) - S_n(z)\}. \tag{3.10.5}$$

Now (3.10.3) produces a useful identity:

$$\log \Gamma(z) = (z - \tfrac{1}{2})\log z - z + \rho(z) + 1 - \rho(1). \tag{3.10.6}$$

It should be noted that $\log \Gamma(z)$ does not necessarily represent the principal value of the logarithm. As a matter of fact the right-hand-side depends continuously on z, and is real if $z > 0$ ($\log z$ s given its principal value). Therefore, (3.10.6) represents the analytic continuation of $\log \Gamma(z)$ throughout the region $|\arg z| < \pi$, starting from real values on the positive real axis.

It is easy to derive an asymptotic formula from (3.10.6), when $|z| \to \infty$. Let δ be a positive constant ($\delta < \pi$), and let R_δ denote the part of the complex plane which is defined by $|\arg z| < \pi - \delta$. Let m be a given integer ≥ 1. Then $B_{2m}(x - [x])$ is bounded, whence

$$\left| \int_0^\infty (z+x)^{-2m}(2m)^{-1}B_{2m}(x-[x])dx \right| < C \int_0^\infty |z+x|^{-2m}dx =$$
$$= C|z|^{-2m+1} \int_0^\infty |y + (z|z|^{-1})|^{-2m}dy,$$

C not depending on z. Now $|y + (z|z|^{-1})|$ represents the distance from the point $-y$ to a point of the unit circle, belonging to the region R_δ. It is easy to see geometrically that this distance is at least $|y + e^{i(\pi-\delta)}|$. Since $\int_0^\infty |y + e^{i(\pi-\delta)}|^{-2m}dy$ converges, we infer that the integral in (3.10.2) is $O(|z|^{1-2m})$. As m is arbitrary, we obtain an asymptotic series for $\rho(z)$, and (3.10.6) gives

$$\log \Gamma(z) - (z - \tfrac{1}{2})\log z + z \approx 1 - \rho(1) + \sum_{k=1}^{\infty} z^{1-2k}(2k)^{-1}(2k-1)^{-1}B_{2k} \quad (|\arg z| < \pi - \delta,\ |z| \to \infty). \tag{3.10.7}$$

It remains to be shown that the constant $1 - \rho(1)$ equals $\frac{1}{2}\log(2\pi)$. We know already that $1 - \rho(1)$ is real, so it suffices to show that $e^{1-\rho(1)} = (2\pi)^{\frac{1}{2}}$. We quote a number of possible methods. (i) In sec. 3.7 it was done with the aid of the Riemann ζ-function, but this is certainly not the most elementary way. (ii) We can use the functional equation $\Gamma(z)\Gamma(-z) = -\pi(z \sin z)^{-1}$, and make z tend to infinity along the imaginary axis. (iii) We can use the functional equation [1])

$$\Gamma(z)\Gamma(z + \tfrac{1}{2}) = \pi^{\frac{1}{2}}2^{1-2z}\Gamma(2z),$$

making $z \to +\infty$. (iv) We can evaluate $\rho(1)$ by evaluation of the integral $\int_0^\infty (1+x)^2B_2(x-[x])dx$. (v) We can use the beginning of sec. 4.5, with $z \to +\infty$.

---

[1]) See E. T. Whittaker and G. N. Watson, Modern Analysis, 4th ed., Cambridge 1946, § 12.15.

3.11. Alternating sums

An alternating sum is a sum of the type $\sum (-1)^k f(k)$, where the $f(k)$ are positive. We usually expect such sums to be small, that is to say, much smaller than the sum of the absolute values of the terms.

We can of course write

$$\sum_{k=0}^{2m+1} (-1)^k f(k) = \sum_{k=0}^{m} f(2k) - \sum_{k=0}^{m} f(2k+1),$$

and investigate both sums on the right. Usually these sums will be about equal, whence it is desirable to study them quite closely in order to have sufficient information about their difference.

In most cases, however, the easiest thing to do, is to take pairs of terms together:

$$\sum_{k=0}^{2m+1} (-1)^k f(k) = \sum_{k=0}^{m} \{f(2k) - f(2k+1)\},$$

and these terms $f(2k) - f(2k+1)$ will usually be small.

As an example we take the infinite sum

$$S(t) = \sum_{k=0}^{\infty} (-1)^k f(k), \quad f(x) = (x^2 + t^2)^{-\frac{1}{2}}, \tag{3.11.1}$$

and we ask for the asymptotic behaviour of $S(t)$ as $t \to \infty$. The function $f(x)$ is decreasing, and tends to zero as $x \to \infty$. Therefore the series converges, and we have, by a well-known theorem on alternating series, $0 < S(t) < f(0)$. Thus a rough first result is that $S(t) = O(t^{-1})$.

We next write

$$S(t) = \sum_{k=0}^{\infty} \{f(2k) - f(2k+1)\}.$$

We shall, of course, compare the difference $f(2k+1) - f(2k)$ with $f'(2k)$, and after that, we shall compare the sum $-\sum_0^\infty f'(2k)$ with the integral $-\frac{1}{2}\int_0^\infty f'(x)dx$ (the factor $\frac{1}{2}$ arises because $2k$ only runs through the even numbers). We can carry out these two operations at the same time, comparing

$$f(2k) - f(2k+1) \quad \text{with} \quad -\tfrac{1}{2}\int_{2k}^{2k+2} f'(x)dx.$$

Using the Taylor series, we can express both in terms of $f(2k)$, $f'(2k), \ldots$. If we stop the Taylor developments at the terms involving f'', i.e. if we apply the formula

$$\varphi(a+h) - \varphi(a) = h\varphi'(a) + \int_a^{a+h} (a+h-x)\varphi''(x)dx,$$

then we obtain

$$f(2k+1) - f(2k) = f'(2k) + \int_{2k}^{2k+1} (2k+1-x)f''(x)dx,$$

$$\tfrac{1}{2}\int_{2k}^{2k+2} f'(x)dx = f'(2k) + \tfrac{1}{2}\int_{2k}^{2k+2} (2k+2-x)f''(x)dx.$$

On subtraction we find

$$f(2k) - f(2k+1) + \tfrac{1}{2}\int_{2k}^{2k+1} f'(x)dx = \tfrac{1}{2}\int_{2k}^{2k+2} (1-|x-2k-1|)f''(x)dx,$$

and so

(3.11.2) $$|f(2k) - f(2k+1) + \tfrac{1}{2}\int_{2k}^{2k+2} f'(x)dx| \le \tfrac{1}{2}\int_{2k}^{2k+2} |f''(x)|dx.$$

In our case we have $f(x) \to 0$ when $x \to \infty$, and therefore

$$\sum_{k=0}^{\infty} \int_{2k}^{2k+2} f'(x)dx = \int_0^{\infty} f'(x)dx = -f(0).$$

It follows that

(3.11.3) $$|S(t) - \tfrac{1}{2}f(0)| \le \tfrac{1}{2}\int_0^{\infty} |f''(x)|dx.$$

We have $f''(x) = (2x^2 - t^2)/(x^2+t^2)^{5/2}$. We transform the integral, substituting $x = yt$:

$$\int_0^{\infty} |f''(x)|dx = t^{-2}\int_0^{\infty} |1-2y^2|/(1+y^2)^{5/2}dy,$$

and the latter integral is easily seen to be convergent. Therefore, (3.11.3) gives

(3.11.4) $$S(t) = \tfrac{1}{2}t^{-1} + O(t^{-2}) \qquad (t \to \infty).$$

The process which led to (3.11.2), can of course be continued: in the next step we use the Taylor expansions up to the terms involving $f'''(x)$. And in order to eliminate the term involving $f''(2k)$, we subtract a suitable multiple of $\int_{2k}^{2k+2} f''(x)dx$, in the same way as we eliminated $-f'(2k)$ by subtracting $-\frac{1}{2}\int_{2k}^{2k+2} f'(x)dx$. This time we use the formula

$$\varphi(a+h) = \varphi(a) + h\varphi'(a) + \tfrac{1}{2}h^2\varphi''(a) + \int_a^{a+h} \tfrac{1}{2}(a+h-x)^2\varphi'''(x)dx,$$

and we obtain

(3.11.5) $$|f(2k) - f(2k+1) + \tfrac{1}{2}\int_{2k}^{2k+2} f'(x)dx - \tfrac{1}{4}\int_{2k}^{2k+2} f''(x)dx| \le$$
$$\le C\int_{2k}^{2k+2} |f'''(x)|dx.$$

As $\int_0^\infty f''(x)dx = -f'(0) = 0$, we now obtain, in the same way as above,

(3.11.6) $$S(t) = \tfrac{1}{2}t^{-1} + O(t^{-3}) \qquad (t \to \infty).$$

There is no term with t^{-2}, and in the next steps of the proceduce it will turn out that the coefficients of $t^{-3}, t^{-4}, \ldots$ vanish also. In order to show this, it is easier to put the series in the following form:

$$S(t) = \tfrac{1}{2}t^{-1} + \tfrac{1}{2}\sum_{k=-\infty}^{\infty} (-1)^k f(k).$$

Applying (3.11.5) to $\Sigma_{-\infty}^{\infty}$, we obtain, as $t \to \infty$,

$S(t) - \frac{1}{2}t^{-1} = -\frac{1}{2}\int_{-\infty}^{\infty} f'(x)dx - \frac{1}{4}\int_{-\infty}^{\infty} f''(x)dx + O(\int_{-\infty}^{\infty} f'''(x)dx)$.

Since $f(x) \to 0$, $f'(x) \to 0$, $f''(x) \to 0$, ... as $x \to \pm\infty$, we have

$$\int_{-\infty}^{\infty} f'(x)dx = \int_{-\infty}^{\infty} f''(x)dx = \int_{-\infty}^{\infty} f'''(x)dx = \ldots = 0.$$

Furthermore it is easily seen, by substitution of $x = yt$, that

$$\int_{-\infty}^{\infty} |f^{(m)}(x)|dx = O(t^{-m}) \qquad (t \to \infty)$$

for every fixed $m > 0$. Now it is sufficient to have only a general idea about the continuation of the process which led to (3.11.4) and (3.11.6) in order to see that

(3.11.7) $$S(t) \approx \tfrac{1}{2}t^{-1} + 0\cdot t^{-2} + 0\cdot t^{-3} + 0\cdot t^{-4} + \ldots \qquad (t \to \infty).$$

It may be remarked that the general formula of which (3.11.2), (3.11.5) are special cases, is related in a trivial way to the Boole sum formula [1]), which we shall not discuss here.

[1]) See C. JORDAN, Calculus of Finite Differences, 2nd ed., New York 1947, § 112.

A second remark is that (3.11.7) can also be derived by the Euler-Maclaurin sum formula, applied separately to $\Sigma f(2k)$ and to $\Sigma f(2k+1)$.

With (3.11.7) we have the same situation as in sec. 3.9. We expect $S(t) - \frac{1}{2}t^{-1}$ to be exponentially small, and by a careful inspection of the above argument, including estimates holding uniformly in m and t, we might be able to show this, although the formulas become quite awkward. But even then we would have only an upper estimate for $S(t) - \frac{1}{2}t^{-1}$, and no asymptotic formula, like the one we shall derive in sec. 3.12.

3.12. Application of the Poisson sum formula

The formula reads

$$\sum_{k=-\infty}^{\infty} f(k+a) = \Sigma_\nu^* e^{2\pi\nu i a} \int_{-\infty}^{\infty} e^{-2\pi\nu i y} f(y)\,dy, \tag{3.12.1}$$

where a is a real number, $f(x)$ is Riemann integrable over any finite interval, and

$$\Sigma_\nu^* \text{ denotes } \lim_{N\to\infty} \sum_{\nu=-N}^{N}.$$

The following set of conditions is easily seen to be sufficient[1]:

(i) $\Sigma_{k=-\infty}^{\infty} f(k+x)$ converges uniformly for $0 \le x \le 1$.

(ii) The function $\phi(x) = \Sigma_{-\infty}^{\infty} f(k+x)$, which has period 1, satisfies the Fourier conditions (that is, $\phi(x)$ is the sum of its Fourier series), at least at $x = a$.

For, condition (i) enables us to carry out the following operation with the Fourier coefficients of $\phi(x)$. If ν is any integer, then the ν-th Fourier coefficient of ϕ equals

$$\int_0^1 e^{-2\pi\nu i y}\phi(y)\,dy = \int_0^1 \sum_{k=-\infty}^{\infty} e^{-2\pi\nu i y} f(k+y)\,dy = \sum_{k=-\infty}^{\infty} \int_0^1 =$$

$$= \sum_{k=-\infty}^{\infty} \int_k^{k+1} e^{-2\pi\nu i y} f(y)\,dy = \int_{-\infty}^{\infty} e^{-2\pi\nu i y} f(y)\,dy.$$

[1]) See for other sets of sufficient conditions: E. C. Titchmarsh, Fourier Integrals, 2nd ed., Oxford 1948, ch. 2.

The last step is legitimate, as (i) implies that

$$\int_k^{k+t} e^{-2\pi\nu i y} f(y)\,dy \to 0$$

when $k \to \pm\infty$, uniformly in $0 \le t \le 1$.

The following set of conditions can be shown to imply (i) and (ii):

(iii) $\Sigma_{-\infty}^{\infty} f(k+a)$ converges,

(iv) $f'(x)$ exists $(-\infty < x < \infty)$,

(v) $\Sigma_{-\infty}^{\infty} f'(k+x)$ converges uniformly in $0 \le x \le 1$.

For, (iii)+(v) imply (i) (apply the mean value theorem to finite sums $\Sigma_N^M f(k+x)$, with M and N either both positive and large or both negative and large), and (v) shows that $\phi(x)$ is differentiable everywhere, whence it satisfies the Fourier conditions.

Another set of sufficient conditions is (iii)+(vi)+(vii), where

(vi) $f(x)$ has bounded variation[1]) over $-\infty < x < \infty$,

(vii) $\lim_{h\to 0} \{f(x+h) + f(x-h)\} = 2f(x)$, at least for all x of the form $a+n$, where n is any integer.

We remark that from (iii)+(vi) one can deduce (i)[2]), as well as the fact that $\phi(x)$ has bounded variation over $0 \le x \le 1$; (vi)+(vii) can be used to show that

$$\lim_{h\to 0} \{\phi(a+h) + \phi(a-h)\} = 2\phi(a).$$

This formula, in combination with the fact that $\phi(x)$ has bounded variation, leads again to (ii).

As it is not our present aim to develop Fourier theory here, we leave it at these brief remarks.

We shall apply the Poisson formula to the sum

$$S_1(t) = \sum_{k=-\infty}^{\infty} f(k), \qquad f(x) = e^{\pi i x}(x^2+t^2)^{-\frac{1}{2}}, \tag{3.12.2}$$

which is related to (3.11.1) by the formula

$$S(t) = \tfrac{1}{2}t^{-1} + \tfrac{1}{2}S_1(t). \tag{3.12.3}$$

The number a occurring in (3.12.1) will be given the special value 0 here, and, in applying (3.12.1) to (3.12.2), t is considered to be a fixed positive number.

[1]) See for definition of bounded variation: E. C. Titchmarsh, Theory of Functions, 2nd ed., Oxford 1939, § 11.4.

[2]) Ibid., § 13.232.

The condition (vi) is not satisfied, but the set (iii)+(iv)+(v) is. Condition (iii) was already checked in the beginning of sec. 3.11, and (iv) is trivial. In order to show (v), we write

$$f'(x) = \pi i e^{\pi i x}(x^2 + t^2)^{-\frac{1}{2}} - x e^{\pi i x}(x^2 + t^2)^{-3/2}.$$

We take two positive integers N, M, where $t < N < M$, and a real number x in $0 \le x \le 1$. Then we consider

$$\sum_{k=N}^{M} f'(x+k) =$$

$$= e^{\pi i x} \sum_{k=N}^{M} (-1)^k \{\pi i((x+k)^2 + t^2)^{-\frac{1}{2}} - (x+k)((x+k)^2 + t^2)^{-3/2}\}.$$

The numbers $\{(x+k)^2 + t^2\}^{-\frac{1}{2}}$ form a decreasing sequence of $(M - N + 1)$ positive numbers, and the same thing holds for $(x+k)\{(x+k)^2 + t^2\}^{-3/2}$. (The function $y(y^2+t^2)^{-3/2}$ decreases from $y = 2^{-\frac{1}{2}}t$ onward). We now use the following well-known fact: If any sequence $a_N, \ldots, a_M$ satisfies $a_N > a_{N+1} > \ldots > a_M > 0$, then we have

$$|\sum_{k=N}^{M} (-1)^k a_k| \le a_N.$$

It follows that

$$|\sum_{k=N}^{M} f'(x+k)| \le (N^2 + t^2)^{-\frac{1}{2}} + N(N^2+t^2)^{-3/2} < 2N^{-1}.$$

As this holds uniformly in x $(0 \le x \le t)$, we infer that, for t fixed, $\sum_1^\infty f'(x+h)$ converges uniformly in $0 \le x \le 1$. The same thing can be said about $\sum_{-\infty}^{0}$, and so we have proved (v).

We can now apply (3.12.1) to (3.12.2); the result is that

$$S_1(t) = \sum_{\nu=-\infty}^{\infty *} \int_{-\infty}^{\infty} e^{-2\pi\nu i y + \pi i y}(y^2 + t^2)^{-\frac{1}{2}} dy, \tag{3.12.4}$$

and so we have to study, for $b = \pm\pi, \pm 3\pi, \pm 5\pi, \ldots$, the integral

$$\int_{-\infty}^{\infty} e^{biy}(y^2 + t^2)^{-\frac{1}{2}} dy.$$

On substitution of $y = tz$ we observe that this integral is a function of bt, to be denoted by φ:

$$\varphi(bt) = \int_{-\infty}^{\infty} e^{btiz}(z^2+1)^{-\frac{1}{2}} dz, \tag{3.12.5}$$

and by substitution of $z = -w$ we infer that φ is an even function. The integral is a Bessel function of zero order, of second kind and of

imaginary argument, and in the standard notation [1])

$$\varphi(bt) = 2K_0(bt).$$

We shall, however, not explicitly use the theory of Bessel functions here.

Using Cauchy's theorem, the integral (3.12.5) can be transformed. Assuming $b > 0$, we deform the integration path $(-\infty, \infty)$ into a new one, consisting of the following parts: (i) The line $(-\infty, -R)$, where R is a large positive number; (ii) The circular arc $z = Re^{i\vartheta}$ $(\pi \ge \vartheta \ge \frac{1}{2}\pi)$; (iii) The segment $z = is$ $(R \ge s \ge 1 + \delta)$, where δ is a small positive number; (iv) The circle $z = i + \delta e^{i\vartheta}$ $(\frac{1}{2}\pi \le \vartheta \le \frac{5}{2}\pi)$; (v) The segment $z = is$ $(1 + \delta \le s \le R)$; (vi) The arc $z = Re^{i\vartheta}$ $(\frac{1}{2}\pi \ge \vartheta \ge 0)$; (vii) The interval (R, ∞). Along (iii), the function $(1+z^2)^{-\frac{1}{2}}$ has to be interpreted as $i(s^2-1)^{-\frac{1}{2}}$, where $(s^2-1)^{\frac{1}{2}}$ is the positive root, and along (v) it has to be interpreted as $-i(s^2-1)^{-\frac{1}{2}}$. Now making $R \to \infty$, $\delta \to 0$ we infer that

$$\varphi(bt) = 2\int_1^\infty e^{-bts}(s^2-1)^{-\frac{1}{2}} ds = 2e^{-bt}\int_0^\infty e^{-btu}(u^2+2u)^{-\frac{1}{2}} du.$$

(The latter integral is obtained from the former by the substitution $s = u + 1$). We have, if $t > 1$, $b \ge \pi$

$$\int_0^\infty e^{-btu}(u^2+2u)^{-\frac{1}{2}} du < \int_0^\infty e^{-\pi u}u^{-\frac{1}{2}} du = 1,$$

and so $|\varphi(bt)| < 2e^{-bt}$ $(b \ge \pi, t \ge 1)$. By (3.12.4) we now have

$$|S_1(t) - 2\varphi(\pi t)| \le |2\varphi(3\pi t) + 2\varphi(5\pi t) + \ldots| \le 2e^{-3\pi t}/(1 - e^{-2\pi t}),$$

and therefore

$$S_1(t) = 2\varphi(\pi t) + O(e^{-3\pi t}) \qquad (t \to \infty). \tag{3.12.6}$$

It remains to find the asymptotic behaviour of $\varphi(\pi t)$. To this end we write, putting $u = x^2$,

$$\varphi(\pi t) = 2e^{-\pi t}\int_0^\infty e^{-\pi t u}(u^2+2u)^{-\frac{1}{2}} du = 2e^{-\pi t}\int_{-\infty}^{\infty} e^{-\pi t x^2}(x^2+2)^{-\frac{1}{2}} dx,$$

in order to be able to apply the method of sec. 4.1. The result is

[1]) See G. N. Watson, Theory of Bessel Functions, 2nd ed., Cambridge 1952, § 6.16.

(cf. the derivation of (4.1.10))

$$\varphi(\pi t) \approx 2e^{-\pi t}(2\pi t)^{-\frac{1}{2}} \sum_{n=0}^{\infty} d_n \Gamma(n+\tfrac{1}{2})\pi^{-n}t^{-n} \qquad (t \to \infty),$$

where the coefficients d_n are those of

$$(2+x^2)^{-\frac{1}{2}} = 2^{-\frac{1}{2}} \sum_{n=0}^{\infty} d_n x^{2n} \quad (|x^2| < 2).$$

For every M the term $O(e^{-3\pi t})$ in (3.12.6) is $O(e^{-\pi t}t^{-\frac{1}{2}-M})$, and therefore $S_1(t)$ has, apart form the factor 2, the same asymptotic power series expansion as $\varphi(\pi t)$. So our final result is, as $d_n = (-1)^n 2^{-3n}(2n)!(n!)^{-2}$:

$$S(t) - \tfrac{1}{2}t^{-1} = \tfrac{1}{2}S_1(t) \approx$$
$$\approx e^{-\pi t} \sum_{n=0}^{\infty} (-1)^n t^{-n-\frac{1}{2}} 2^{\frac{1}{2}-5n} \pi^{-n} \{(2n)!\}^2 \{n!\}^{-3} \quad (t \to \infty).$$

3.13. Summation by parts

We often meet the question of the asymptotic behaviour, as $n \to \infty$, of a sum $a_1 b(1) + \ldots + a_n b(n)$, where the behaviour of $a_1 + \ldots + a_n$ is known and where the function $b(x)$ behaves smoothly. Then we can usually apply the formula for summation by parts:

(3.13.1) $$a_1 b_1 + \ldots + a_n b_n = A_1(b_1 - b_2) + A_2(b_2 - b_3) + \ldots + A_{n-1}(b_{n-1} - b_n) + A_n b_n,$$

where $A_k = a_1 + a_2 + \ldots + a_k$, and b_k is an abbreviation for $b(k)$. It has some formal advantages to write the formula in terms of integrals. We assume, for simplicity, that $b(x)$ has a continuous derivative, and we put $A(x) = \sum_{1 \le m \le x} a_m$ (i.e. $A(x) = 0$ if $x < 1$, $A(x) = a_1 + \ldots + a_k$ if $k \le x < k+1$ $(k = 1, 2, \ldots)$). Then (3.13.1) becomes

(3.13.2) $$a_1 b(1) + \ldots + a_n b(n) = A(n)b(n) - \int_1^n A(x)b'(x)dx.$$

As an example we consider the sum $\sum_{k=1}^n \sin(kt)\log k$, where t is a real constant. We put $\sin kt = a_k$, $\log x = b(x)$. For every n we have

$$\sum_{k=1}^n \sin kt = \operatorname{Im} \sum_{k=1}^n e^{ikt} = \operatorname{Im}\{(e^{i(n+1)t} - e^{it})/(e^{it} - 1)\}.$$

Therefore, there is a number $C > 0$, not depending on n, such that $|\sum_1^n \sin kt| < C$. (If $e^{it} - 1 = 0$, our argument fails, but the result still holds, for then $\sin kt = 0$ for all k). Putting $A(x) = \sum_{1 \le k \le x} \sin kt$, we have, by (3.13.2),

$$\sum_{k=1}^n \sin(kt)\log k = A(n)\log n - \int_1^n A(x)x^{-1}dx.$$

Since $|A(x)| < C$ for all x, we now easily derive that

$$\sum_{k=1}^n \sin(kt)\log k = O(\log n) \quad (t \text{ fixed}, n \to \infty).$$

We shall discuss a second example, taken from the theory of primes. We take $a_n = \log n$ if n is a prime number, and $a_n = 0$ otherwise. Then $A(x)$ is the function usually denoted by $\vartheta(x)$, and we can write

$$\vartheta(x) = \sum_{p \le x} \log p.$$

It is a fundamental and far from trivial result of the theory of primes that, for each m $(m = 1, 2, 3, \ldots)$, we have [1]

(3.13.3) $$\vartheta(x) = x + O(x(\log x)^{-m}) \quad (x \to \infty).$$

Now many other sums involving primes, as $\sum_{p \le x} p^{-1}$, $\sum_{p \le x} p^2$, $\sum_{p \le x} 1$, can be dealt with. We consider $\sum_{p \le x} 1$, i.e. the number of primes not exceeding x. This number is usually denoted by $\pi(x)$. We have, by (3.13.2), taking $b(x) = (\log x)^{-1}$,

$$\pi(n) = a_2 b(2) + \ldots + a_n b(n) =$$
$$= (\log n)^{-1}\vartheta(n) - \int_2^n \vartheta(x)d(\log x)^{-1}.$$

(We have replaced the lower limit 1 by 2, since $(\log x)^{-1}$ is singular at $x = 1$; it makes no difference, as $\vartheta(1) = 0$). We compare this with

$$\int_2^n (\log x)^{-1}dx = [x(\log x)^{-1}]_2^n - \int_2^n x\,d(\log x)^{-1}.$$

On subtraction we obtain, using (3.13.3),

$$\pi(n) - \int_2^n (\log x)^{-1}dx = (\log n)^{-1}O(n(\log n)^{-m}) +$$
$$+ \int_2^n O(x(\log x)^{-m})(\log x)^{-2}x^{-1}dx \qquad (n \to \infty).$$

[1] See A. E. Ingham, The Distribution of Primes, Cambridge 1932, p. 12 and p. 63.

The integral on the right can be written as

$$\int_2^{n^{\frac{1}{2}}} O(1)dx + \int_{n^{\frac{1}{2}}}^{n} O\{(\log n^{\frac{1}{2}})^{m-2}\}dx = O(n(\log n)^{-m-2}) \qquad (n \to \infty),$$

and therefore

$$\pi(n) - \int_2^n (\log x)^{-1}dx = O(n(\log n)^{-m-1}) \qquad (n \to \infty).$$

The integral on the left can easily be expanded in the form of an asymptotic series (cf. (1.5.5)), and we infer that

$$\pi(n) \approx n \log^{-1} n + n \log^{-2} n + 2!n \log^{-3} n + \\ + 3!n \log^{-4} n + \dots \qquad (n \to \infty).$$

Meanwhile we notice that (3.13.3) is an example of the situation described in secs. 3.9 and 3.11. Again there is an asymptotic expansion with zero coefficients:

$$e^{-x}\vartheta(e^x) - 1 \approx 0\cdot x^{-1} + 0\cdot x^{-2} + 0\cdot x^{-3} + \dots \qquad (x \to \infty),$$

but in this case the question as to whether the left hand side is exponentially small, is still unsolved.

3.14. Exercises. 1. Show (e.g. by the method of summation by parts) that

$$\sum_{n=1}^{\infty} n^{-1}e^{-n^2t} = -\tfrac{1}{2}\log t + \tfrac{1}{2}\gamma + O(t^{\frac{1}{2}}) \qquad (0 < t < 1),$$

where $\gamma = -\int_0^\infty e^{-x}\log x\, dx$ is Euler's constant.

2. Show that

$$\sum_{n=0}^{\infty} \log(1 - be^{-nt}) \approx c_{-1}t^{-1} + c_0 + c_1t + c_2t^2 + \dots \qquad (t > 0, t \to 0).$$

Here b is a constant, $0 < b < 1$, and

$$c_k = (-1)^k (B_{k+1}/(k+1)!) \sum_{n=1}^{\infty} b^n n^{k-1} \qquad (k = -1, 0, 1, 2, \dots).$$

3. Show that

$$\sum_{n=1}^{\infty} \log(1 - e^{-nt}) \approx -\pi^2/(6t) - \tfrac{1}{2}\log t + \tfrac{1}{2}\log(2\pi) + \tfrac{1}{24}t + \\ + 0\cdot t^2 + 0\cdot t^3 + \dots \qquad (t > 0, t \to 0).$$

(Hint: Apply the Euler-Maclaurin formula to $\Sigma_0^N f(n)$, where

$$f(x) \triangleq \log\{(1 - e^{-xt})/xt\}).$$

4. Let s_n be defined by

$$s_n = \frac{1}{\log n} - \frac{1}{\log(n+1)} + \frac{1}{\log(n+2)} - \dots .$$

Show that

$$s_n = \tfrac{1}{2}(\log n)^{-1} + O(n^{-1}\log^{-2} n) \qquad (n \to \infty).$$

5. Derive from (3.13.3) that

$$\Sigma_p e^{-pt} \approx -\sum_{n=0}^{\infty} t^{-1}(\log t)^{-n-1}\int_0^\infty e^{-y}(\log y)^n dy \qquad (t > 0,\ t \to 0),$$

if the summation variable p runs through all prime numbers (cf. sec. 1.8, exerc. 4).