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ON SUMMATION FORMULAS DUE TO PLANA, LINDELÖF AND ABEL, AND RELATED GAUSS-CHRISTOFFEL RULES, II *

GERMUND DAHLQUIST

[1] *NADA, Royal Institute of Technology, S 10044 Stockholm, Sweden*
email: consim@nada.kth.se

Abstract.

This part contains Chapter 3 (of 5), which is mainly concerned with the derivation, analysis and applications of a summation formula, due to Lindelöf, for alternating series and complex power series, including ill-conditioned power series. An appendix is devoted to complete monotonicity and related questions.

The reader is referred to Part I (in this volume of BIT) for the abstract, the contents and the bibliography of the whole work. A short list of references for this part is at the end of this part.

3 The Lindelöf summation formula.

3.1 Derivation of the summation formula, the Fourier transform and the moments.

Let C be a closed rectangular contour with vertices at $(m-\frac{1}{2}-i\Omega)$, $(n+\frac{1}{2}-i\Omega)$, $(n+\frac{1}{2}+i\Omega)$, $(m-\frac{1}{2}+i\Omega)$, and consider the integral

$$I = \frac{1}{2\pi i}\int_C \frac{\pi f(s)}{\sin \pi s}\, ds.$$

Most texts on Complex Analysis consider the case where $\Omega = n+\frac{1}{2}$, $m=-n$ and $f(s)$ is regular in the whole plane, except for a finite number of poles $\{p_j\}$. Moreover, they assume that $|f(s)| = O(|s|^{-2})$ as $|s| \to \infty$, so that $I \to 0$ as $n \to \infty$. For example, if the poles are non-integers and simple, we have by the residue theorem as $n \to \infty$,

$$\sum_{k=-\infty}^{\infty} (-1)^k f(k) = -\sum_j \pi \operatorname{res}_f(p_j)/\sin \pi p_j.$$

Let

$$s = \sigma + i\omega; \quad m^* = m - \tfrac{1}{2}.$$

Consider again the contour integral I, but following Lindelöf [9, 1905], we shall

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make a different set of *assumptions*, in order to derive Eq. (3.1) (which is equivalent to alternative L in (1.10)).

(a) $f(s)$ is analytic in the *half-plane*, $\sigma \geq m - \frac{1}{2}$. ($f(s)$ is not assumed to be analytic at ∞.)

(b) $\lim_{\omega \to \pm\infty} e^{-\pi|\omega|} f(\sigma + i\omega) = 0$, uniformly in every strip $\sigma \in [m - \frac{1}{2}, n + \frac{1}{2}]$, $m < n$.

(c) $\lim_{\sigma \to \infty} \int_{-\infty}^{\infty} e^{-\pi|\omega|} |f(\sigma + i\omega)| \, d\omega = 0$.

In this case, $I = \sum_{k=m}^{n} (-1)^k f(k)$. By Assumption (b), the contributions from the horizontal sides tend to zero, as $\Omega \to \infty$, (for any n). The rectangle becomes a strip. Then, by Assumption (c), the contribution from the right boundary of the strip tends to zero, as $n \to \infty$ through integral values. So, I reduces to the integral along the left boundary of the strip, i.e.,

$$\sum_{k=m}^{\infty} (-1)^k f(k) = \int_{-\infty}^{\infty} \frac{f(m - \frac{1}{2} + i\omega)}{2\sin((m - \frac{1}{2})\pi + \pi i\omega)} \, d\omega.$$

The *Lindelöf summation formula* follows:

$$\sum_{k=m}^{\infty} (-1)^k f(k) = (-1)^m \int_{-\infty}^{\infty} \frac{f(m - \frac{1}{2} + i\omega)}{2\cosh \pi\omega} \, d\omega. \tag{3.1}$$

It is important that we have obtained an integral with a positive weight function called the *Lindelöf density* and denoted $w^L(\omega) = 1/(2\cosh \pi\omega)$ that does not depend on f and m. This form of the Lindelöf summation formula is easier to handle for theoretical discussions than the equivalent formula (3.21), which is better for practical computation. (The latter is the same as alternative L in (1.10).)

Suppose that $\sum_{k=1}^{\infty}$ is to be computed. It is most common to choose $m \geq 1$, but for the applications to a power series the choice of a non-positive m is occasionally useful. With the convention $\sum_{1}^{0} \ldots = 0$, we have

$$\sum_{1}^{\infty} = \sum_{1}^{m-1} + \sum_{m}^{\infty}, \ m \geq 1, \quad \sum_{1}^{\infty} = -\sum_{m}^{0} + \sum_{m}^{\infty}, \ m \leq 0. \tag{3.2}$$

The application of (3.1) to the case $f(s) = e^{-ts}$ yields, after some simplification, the *Fourier transform* of the Lindelöf density and some other relevant old results,

$$\frac{1}{2\cosh t/2} = \frac{e^{t/2}}{e^t + 1} = \int_{-\infty}^{\infty} \frac{e^{-i\omega t}}{2\cosh \pi\omega} \, d\omega = \sum_{p=0}^{\infty} \frac{\mu_p (-it)^p}{p!}, \tag{3.3}$$

where μ_p are the *moments* of the relevant weight function,

$$\mu_p = \int_{-\infty}^{\infty} \frac{\omega^p}{2\cosh \pi\omega} \, d\omega. \tag{3.4}$$

(By symmetry, the moments of odd order are zero.) This indicates a connection with the *Euler numbers* E_n defined by the generating function

$$\frac{1}{\cosh t/2} = \sum_{p=0}^{\infty} \frac{E_p}{p!}\left(\frac{t}{2}\right)^p, \tag{3.5}$$

see, e.g., Abramowitz and Stegun, [1, Sec. 23.1]. It follows that $E_0 = 1$, $E_2 = -1$, $E_4 = 5$, $E_6 = -61$,

$$\mu_{2k} = 2^{-2k-1}|E_{2k}|, \quad \operatorname{sign} E_{2k} = (-1)^k, \quad E_{2k+1} = 0, \quad E_k = |E_k| i^k. \tag{3.6}$$

In particular, $\mu_0 = 1/2$.

An asymptotic formula for the Euler numbers is given in (3.16). The application of the Krylov algorithm (2.42) or (2.40) to Eq. (3.8) is *a convenient way to compute the Euler numbers.* See §4.1 about a similar computation of the Bernoulli numbers.

A curious spin-off: by a simple change of variables in (3.3), we find that $1/\cosh(t\sqrt{\pi/2})$ is an eigenfunction of the Fourier transform belonging to the eigenvalue $\sqrt{2\pi}$. Another eigenfunction to the same eigenvalue is $\exp(-\frac{1}{2}t^2)$. These results will not be used in this paper, but the following simple lemma is fundamental for the next section.

LEMMA 3.1. *The Euler numbers are uniquely determined by a recurrence relation that can be written in "symbolic" form as*

$$E_0 = 1, \quad \Re(|E| + i)^k = 0, \quad k = 1, 2, \ldots,$$

where, after the expansion by the binomial theorem, the power $|E|^p$ should be replaced by $|E_p|$.

PROOF. Write "symbolically"

$$e^{|E|x} = \sum_{k=0}^{\infty} \frac{|E_k| x^k}{k!} = \sum_{k=0}^{\infty} \frac{E_k (ix)^k}{k!} = \frac{1}{\cosh ix} = \frac{1}{\cos x}, \quad x \in \mathbf{R}.$$

We here used (3.6) and (3.5). Hence

$$\frac{e^{ix}}{\cos x} = e^{|E|x} e^{ix} = e^{(|E|+i)x} = \sum_{k=0}^{\infty} \frac{(|E| + i)^k x^k}{k!}.$$

Since $\Re e^{ix}/\cos x \equiv 1$, the sequence of Euler numbers satisfy the recurrence relation. It is evidently the only sequence that satisfies the initial condition $E_0 = 1$ too. Note that the recurrence relation implies the well known fact that the Euler numbers are integers. □

3.2 The three term recurrence relation.

The computation of the matrix $\widehat{J}$ according to Section 2 led to the *conjecture* that $\hat{\beta}_k = \frac{1}{2}k$, i.e.,

$$2\widehat{J} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 1 & 0 & 2 & \dots & 0 & 0 \\ 0 & 2 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & n-1 \\ 0 & 0 & 0 & \dots & n-1 & 0 \end{pmatrix}. \tag{3.7}$$

Recall that $\widehat{J}$ is uniquely determined by the moments μ_k, $0 \le k < 2n$, $\mu_0 = \frac{1}{2}$. By (2.39) and (3.6), this conjecture is therefore equivalent to the equations

$$e_1^T(2\widehat{J})^k e_1 = 2^k \mu_k/\mu_0 = |E_k|, \quad 0 \le k < 2n. \tag{3.8}$$

By Lemma 3.1, it is then equivalent to the equations,

$$\Re e_1^T(2\widehat{J} + iI)^k e_1 = \Re(|E| + i)^k = \begin{cases} 0, & \text{if } 0 < k < 2n, \\ 1, & \text{if } k = 0, \end{cases} \tag{3.9}$$

where the middle expression is "symbolic". We now formulate the conjecture as a theorem and prove it.

THEOREM 3.2. *The three term recurrence relation for the orthonormal polynomials for the Lindelöf density function* $w^L(\omega) = 1/(2\cosh \pi\omega)$ *has the coefficients* $\widehat{\beta}_k = \frac{k}{2}$, $\widehat{\alpha}_k = 0$.

PROOF. Let $\widehat{J}$ be defined by (3.7). By the above discussion it is necessary and sufficient to prove Eq. (3.9). Evidently this is valid for $k = 0$. Consider the Krylov row sequence, $v_k = e_1^T(2\widehat{J} + iI)^k$. We shall show that the real part of the first component $v_k e_1$ is zero for $k = 1, 2, \dots$. We do this for the infinite-dimensional matrix, i.e., $n = \infty$. (For the $n \times n$ principal submatrix of $2\widehat{J}$, $v_k e_1$ is the same, as long as $k < 2n$.)

Note that $v_1 = [i, 1, 0, 0, 0, \dots]$. The following patterns were discovered by numerical experimentation; for some *real* numbers a_j, a'_j, a''_j,

$$\begin{aligned} v_{2m-1} &= [\, ia_1,\ a_1,\ ia_2,\ a_2, \dots], \\ v_{2m} &= [\, 0,\ ia'_1,\ a'_1,\ ia'_2,\ a'_2, \dots], \\ v_{2m+1} &= [\, ia''_1,\ a''_1,\ ia''_2,\ a''_2, \dots]. \end{aligned}$$

Note that the row v_{2m+1} has the same pattern as v_{2m-1}. It will now be proved by induction that this is generally true. Therefore assume that the first formula holds for a certain m; we already know that it holds for $m = 1$. Then consider $v_{2m} = v_{2m-1}(2\widehat{J} + iI)$. The first component equals $a_1 i^2 + a_1 = 0$.

For column $2p$ we obtain $ia'_p = ia_p(2p-1) + a_p i + ia_{p+1}2p$, i.e., $a'_p = 2p(a_p + a_{p+1})$.

For column $2p+1$ we then obtain $a_p 2p + ia_{p+1}i + a_{p+1}(2p+1) = 2p(a_p + a_{p+1})$. So the formula for v_{2m} is true with $a'_p = 2p(a_p + a_{p+1}) \in \mathbf{R}$, $p \ge 1$.

In the same way, if we set $a'_0 = 0$, we find that the formula for $v_{2m+1} = v_{2m}(2\widehat{J} + iI)$ is true with $a''_p = (2p-1)(a'_{p-1} + a'_p) \in \mathbf{R}$.

This completes the induction, and we see that the real part of the first component of v_k is always zero. This proves Eq. (3.9). □

After the theorem had been proved, the writer was informed that the result is not new. It is implicitly contained in an early study of a family of continued fractions, Stieltjes [10, 1889]. Some ideas of Stieltjes and more recent authors are presented in §5.1 and applied to the recursion coefficients for the Abel density.

3.3 A semi-convergent expansion related to the Lindelöf formula.

The relation of the Plana formula to the Euler-Maclaurin expansion was mentioned in the introduction. We shall now consider an expansion that is related to the Lindelöf formula in a similar way. It is mentioned by Lindelöf, [9], p. 78, and a remainder is given on p. 83. Since little attention has been paid to it in the numerical literature, we shall now discuss it. Consider (3.1)

$$\sum_{k=m}^{\infty}(-1)^k f(k) = (-1)^m \int_{-\infty}^{\infty} \frac{f(m^* + i\omega)}{2\cosh \pi\omega}\, d\omega, \quad m^* = m - \frac{1}{2}.$$

Expand $f(m^*+i\omega)$ into powers of ω, with a remainder, and exchange the order of summation and integration. This leads to an expansion $\sum_{k=m}^{\infty}(-1)^{k-m}f(k) = \sum_{\nu=0}^{2q} i^\nu \mu_\nu f^{(\nu)}(m^*)/\nu! + R'_q$, where μ_ν is the moment defined by (3.4). The remainder R'_q will be discussed below. By (3.6),

$$\sum_{k=m}^{\infty}(-1)^{k-m}f(k) = \sum_{p=0}^{q} \frac{E_{2p} f^{(2p)}(m^*)}{2^{2p+1}(2p)!} + R'_q. \tag{3.10}$$

Note that all imaginary quantities have disappeared. Also note that the expansion contains the derivatives of even order, while the Euler-Maclaurin expansion (1.6) contains the derivatives of odd order. This expansion usually diverges as $q \to \infty$, but it is semiconvergent; for large values of m a modest number of terms often yields rather high accuracy. The first coefficients are as follows:

$2p$	0	2	4	6	8	10
E_{2p}	1	-1	5	-61	1385	-50521
$\frac{E_{2p}}{2^{2p+1}(2p)!}$	$\frac{1}{2}$	$\frac{-1}{16}$	$\frac{5}{768}$	$\frac{-61}{92160}$	$\frac{277}{4128768}$	$\frac{-50521}{2^{11}10!}$

The reader may, as a hopefully amusing exercise, apply (3.10) for explaining the following curious observation, see Borwein et al. [2, 1989].

$$\sum_{k=1}^{50} \frac{4(-1)^k}{2k-1} = 3.12159465259\ldots$$

$$\pi = 3.14159265359\ldots.$$

Note that only three digits disagree. There are several variations on this theme. Borwein et al. actually displayed the case with 40 decimal places based on 50,000 terms. You may find out how few digits disagreed.

In this subsection we drop all analyticity assumptions, and this is the main reason for the inclusion of it in this paper. We make instead the following *assumptions.*

(a) The series $\sum_m^\infty (-1)^k f(k)$ is convergent,

(b) All derivatives $f^{(\nu)}(s)$ occurring below exist for $s \geq m^*$, and tend to zero as $s \to \infty$.

(c) All integrals from m^* to ∞ occurring below are absolutely convergent.

Results concerning a finite sum $\sum_{k=m}^{n-1}(-1)^k f(k)$ formally obtained by subtracting an expression for $\sum_{k=n}^{\infty}(-1)^k f(k)$ from the corresponding expression for $\sum_{k=m}^{\infty}(-1)^k f(k)$, are here valid, also if the infinite expansions diverge. (A similar remark was made in the introduction concerning Eq. (1.4).) The derivation of the remainder R_q' is rather analogous to well known derivations concerning the Euler-Maclaurin summation formula. We need some basic properties of the Euler polynomials and the periodic Euler functions. Since this is classical, we omit the details of some straightforward computations.

The *Euler polynomials* $E_n(x)$ are defined by the generating function,

$$\frac{2e^{xy}}{e^y+1} = \sum_{n=0}^{\infty} E_n(x)\frac{y^n}{n!}.$$

The following equations are rather immediate consequences of the generating functions for the Euler polynomials and the Euler numbers:

$$E_n(1-x) = (-1)^n E_n(x), \quad 2^n E_n(\tfrac{1}{2}) = E_n, \tag{3.11}$$

$$E_0(x) = 1, \quad E_{n+1}'(x) = (n+1)E_n(x), \quad E_{2p}(0) = 0, \ (n > 0). \tag{3.12}$$

The *periodic Euler functions* $\bar{E}_n(x)$ are defined by

$$\bar{E}_n(x) = E_n(x) \ (0 < x < 1), \quad \bar{E}_n(x+1) = -\bar{E}_n(x), \ \forall x \in \mathbf{R}.$$

The period is evidently equal to 2. The integral of $E_n(\cdot)$ over a full period is zero. The equations (3.11), (3.12) hold for the periodic Euler functions too, and note that

$$\bar{E}_n(m^*) = (-1)^{m-1}E_n(\tfrac{1}{2}) = 2^{-n}(-1)^{m-1}E_n. \tag{3.13}$$

By (3.12) and (3.13),

$$\int_a^x \frac{\bar{E}_n(t)\,dt}{n!} = \frac{\bar{E}_{n+1}(x) - \bar{E}_{n+1}(a)}{(n+1)!}. \tag{3.14}$$

(This is used below for $a = 0$ or $a = m^*$.) For $n > 0$ the piecewise polynomial $\bar{E}_n(\cdot)$ belongs to $C^{n-1}(\mathbf{R})$. $\bar{E}_n(\cdot)$ is even when n is odd, and vice versa.

$E_0(x) \equiv 1$, hence $\bar{E}_0(x) = (-1)^{\lfloor x \rfloor}$ is "a square wave" with a well known Fourier expansion. By termwise integration of this $2p$ times we obtain, because of (3.14),

$$\bar{E}_{2p}(x) = \frac{(-1)^p 4(2p)!}{\pi^{2p+1}} \sum_{\nu=0}^{\infty} \frac{\sin(2\nu+1)\pi x}{(2\nu+1)^{2p+1}}. \tag{3.15}$$

(A cosine expansion for $\bar{E}_{2p+1}(x)$ can be obtained by one more integration.) We obtain, for $x = \frac{1}{2}$, the following approximate expression for the coefficients of (3.10).

$$\frac{E_{2p}}{2^{2p+1}(2p)!} \sim \frac{2(-1)^p}{\pi^{2p+1}} \quad (p \to \infty). \tag{3.16}$$

For example, when $p = 3$ the right hand side equals $6.622 \cdot 10^{-4}$, while the left hand side (mentioned above) is $61/92160 \approx 6.619 \cdot 10^{-4}$.

After some straightforward calculation, we obtain

$$2 \sum_{k=m}^{\infty} (-1)^k f(k) = -\bar{E}_0(m^*) f(m^*) - \int_{m^*}^{\infty} \bar{E}_0(s) f'(s)\, ds. \tag{3.17}$$

After repeated integrations by parts, and by the use of (3.14), the right hand side becomes

$$-\sum_{j=0}^{q} \frac{\bar{E}_{2j}(m^*) f^{(2j)}(m^*)}{(2j)!} - \int_{m^*}^{\infty} \frac{\bar{E}_{2q}(s) f^{(2q+1)}(s)}{(2q)!}\, ds.$$

We now compare this with (3.10). Notice the factor 2 on the left hand side of (3.17), and recall that $\bar{E}_{2p}(m^*) = 2^{-2p}(-1)^{m-1} E_{2p}$. We then find that the expansions are equivalent, and we conclude that the remainder of (3.10) becomes

$$R'_q = \frac{1}{2}(-1)^{m-1} \int_{m^*}^{\infty} \frac{\bar{E}_{2q}(s) f^{(2q+1)}(s)}{(2q)!}\, ds. \tag{3.18}$$

This is not so useful, since the integral of $\bar{E}_{2q}(s)$ over a period is zero. A more useful form for R'_q is obtained by integrating (3.18) twice by parts,

$$R'_q = \frac{1}{2}(-1)^m \int_{m^*}^{\infty} \frac{\bar{E}_{2q+2}(m^*) - \bar{E}_{2q+2}(s)}{(2q+2)!} f^{(2q+3)}(s)\, ds. \tag{3.19}$$

We shall now see that the error estimation can be much simpler, under certain assumptions, which are often satisfied. It is known that $|\bar{E}_{2p}(s)| \le |\bar{E}_{2p}(m^*)| = |\bar{E}_{2p}(\frac{1}{2})| = |2^{-2p} E_{2p}|$, see, e.g., Abramowitz and Stegun [1], formula 23.1.13, hence

$$|R'_q| \le \frac{2^{-2q}|E_{2q}|}{2(2q)!} \int_{m^*}^{\infty} |f^{(2q+1)}(s)|\, ds \sim \frac{2}{\pi^{2q+1}} \int_{m^*}^{\infty} |f^{(2q+1)}(s)|\, ds. \tag{3.20}$$

It also follows that $\bar{E}_{2p}(m^*) - \bar{E}_{2p}(s)$ has constant sign in $[m^*, \infty]$, the same as $\bar{E}_{2p}(m^*)$. *Suppose* that $f^{(2q+3)}(s)$ has constant sign in the interval (m^*, ∞). Then, by (3.19) and (3.12),

$$\operatorname{sign} R'_q = \operatorname{sign}\big((-1)^{m-1}\bar{E}_{2q+2}(m^*)f^{(2q+2)}(m^*)\big) = \operatorname{sign}\big(E_{2q+2}f^{(2q+2)}(m^*)\big).$$

An important conclusion is that R'_q *has the same sign as the first neglected term on the right hand side of* (3.10), *if* $f^{(2q+3)}(s)$ *has constant sign in the interval* (m^*, ∞). *If we moreover assume that* $f^{(2q+5)}(s)$ *has the same sign as* $f^{(2q+3)}(s)$, $s \geq m^*$, *then* $|R'_q|$ *does not exceed the magnitude of the first neglected term*, for then $\operatorname{sign} R'_q = -\operatorname{sign} R'_{q+1}$, since the Euler numbers have alternating signs.

These assumptions hold for all q when $f(s)$ is *completely monotonic*. Then $f(s)$ is analytic and bounded for $\Re s \geq m^*$, but not necessarily entire, see §3.7.

By (3.20), a sufficient condition for convergence of the expansion to the correct sum as $q \to \infty$ for a fixed m^* is that $f(s)$ is an *entire function*, such that $|f(s)| = O(e^{a|s|})$, $a < \pi$. This is to be looked upon as an almost necessary condition for convergence, although there are exceptional cases, e.g., if $f(s-m^*)$ is an odd function, then all terms in the expansion are zero. In such exceptional cases the remainder may or may not converge to zero, as $q \to \infty$ for a fixed m^*. It can happen that the expansion converges to the wrong result, if the remainder is not taken into account!

This type of convergence is, however, not necessary for the practical use of the expansion. Therefore the expansion can be useful when $f(s)$ is a completely monotonic function that is not an entire function.

For example, take $f(s) = s^{-1}$. By (3.20), the smallest error bound for a given m^* is obtained when $2q \approx \pi m^*$. The error bound, and the true error, are then, by Stirling's formula, about $e^{-\pi m^*}\sqrt{2/m^*}$, which can be made arbitrarily small, *if* m^* *is chosen large enough.* The expansion is semi-convergent.

In practice, since the computation of higher derivatives usually costs much more than the computation of $f(k)$, also with modern methods for automatic differentiation, it is usually better to choose a moderate value of q and to diminish the error by increasing m^*.

Suppose that complex arithmetic is conveniently available and that high accuracy is needed. Unless the computation of derivatives is extremely simple, the writer considers the Gauss-Lindelöf approach, discussed in the following sections, superior to the expansion (3.10), even with optimal m and q. By the way, this remark also applies to the comparison of the Euler-Maclaurin expansion with the Gauss-Plana approach, see Ch. 4.

Finally, it should be mentioned that Lindelöf [9, § 39] has a different representation of the remainder as an integral $\int_{-\infty}^{\infty} p_{2k}(m^*, \omega)w^L(\omega)\,d\omega$, where $p_{2k}(m^*, \omega)$, $k = q+1$ is an integral form for the remainder in Taylor's formula that requires $f^{(2k)}(m^* + iu)$ for $-\omega \leq u \leq \omega$.

3.4 Nodes and weights etc. for the Gauss-Lindelöf rule.

In this section we return to the notations for the Lindelöf formula originally given in (1.10); w^L is called *the Lindelöf density.*

$$
\begin{aligned}
m^* &= m - 1/2, \\
g_\sigma^L(\omega) &= \frac{1}{2}\big(f(\sigma+i\omega)+f(\sigma-i\omega)\big), \quad w^L(\omega) = \frac{1}{2\cosh \pi\omega}, \\
\sum_{k=1}^{\infty}(-1)^{k-1}f(k) &= \sum_{k=1}^{m-1}(-1)^{k-1}f(k) + (-1)^{m-1}\int_{-\infty}^{\infty} g_{m^*}^L(\omega)w^L(\omega)\,d\omega.
\end{aligned} \tag{3.21}
$$

This is equivalent to Eq. (3.1). The last term is called the *Lindelöf integral.* Note that if $f(s)$ is real on the real axis, then $g_{m^*}^L(\omega) = \Re f(m^* + i\omega)$. Recall that, by Theorem 3.2 and (2.17), the recursion coefficients and the leading coefficients are

$$
\widehat{\beta}_n = \frac{n}{2}, \quad A_0 = \mu_0^{-1/2} = \sqrt{2}, \; A_n = \mu_0^{-1/2}\prod_{k=1}^{n}\widehat{\beta}_k^{-1} = \frac{2^{n+1/2}}{n!}, \tag{3.22}
$$

The *error constant* in (2.28) becomes

$$
r_n = \frac{1}{A_n^2(2n)!} = \frac{2^{-2n-1}(n!)^2}{(2n)!} = 2^{-4n-1}\sqrt{\pi n}\left(1+O\left(\frac{1}{n}\right)\right), \tag{3.23}
$$

where the last expression is a useful approximation, obtained by Stirling's formula. For example, if $n = 4$, $r_n = 2.790\cdot 10^{-5}$, while the approximation gives $2.705\cdot 10^{-5}$.

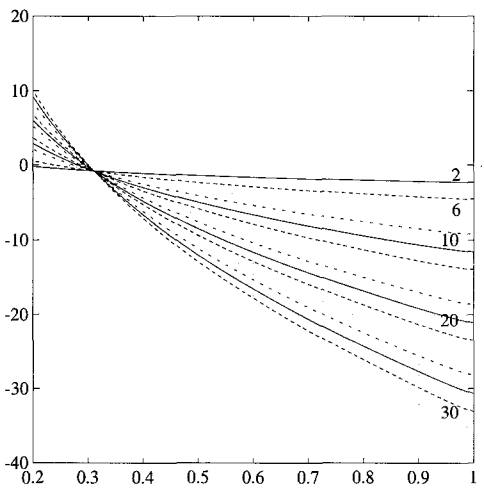

Figure 3.1: $\log_{10} r_n(\alpha)$, according to (2.30), $n = 2 : 2 : 30$.

The *error factor* $r_n(\alpha)$, defined in (2.30), is shown in Fig. 3.1. It was computed for $n = 2 : 2 : 30$ without truncation error by means of the Gauss-Lindelöf rule

with $n = 32$. We have $r_n(1) = r_n$. $r_n(\alpha)$ seems to be of limited practical interest for $\alpha < \frac{1}{3}$.

Put $\bar{\alpha} = \pi(1 - \alpha)$. A preliminary study of Fig. 3.1 indicates that $\log r_n(\alpha) \approx \log r_n + \bar{\alpha}(n + \kappa_1(n)) + \bar{\alpha}^2(0.14n + \kappa_2(n))$, where $\kappa_i'(n) \to 0$ as $n \to \infty$. From the above expression we see that $\log r_n = -4n \log 2 + \kappa_0(n)$, where $\kappa_0'(n) \to 0$ as $n \to \infty$. Then, for $n \gg 1$, $\frac{\partial}{\partial n} \log r_n = 0$ when $-4 \log 2 + \bar{\alpha} + 0.14\bar{\alpha}^2 = 0$. The positive root of this quadratic is $\bar{\alpha} \approx 2.14$, i.e., $\alpha \approx 0.32$. This fits well with the almost-convergence of the pencil of curves in Fig. 3.1 at $\alpha \approx 0.32$. The coefficients of α and α^2 can also be derived from an approximation of $\widehat{\phi}^2(\omega) w^L(\omega)$ for $\omega = n + O(\sqrt{n})$ by a Gauss function, see Fig. 3.2.

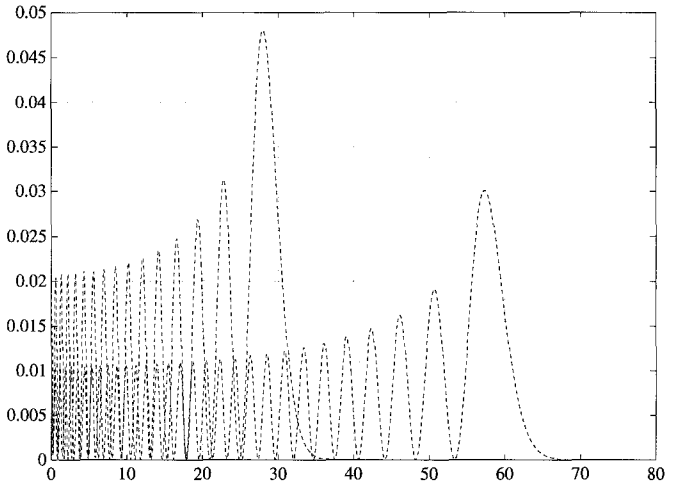

Figure 3.2: $\widehat{\phi}_n^2(\omega) w^L(\omega)$ versus ω for $n = 30$ and $n = 60$.

Before the writer had found the explicit expression for the recursion coefficients β_n, the power basis was tried. The Cholesky factorization $R^T R = G$ was computed with the shortcuts of §2.4. By (2.20), $\beta_i = r_{i+1,i+1}/r_{i,i}$. The β_i were obtained exactly for $i \leq 11$; afterwards the logarithm of the relative error of β_i grew almost linearly, until the Cholesky factorization broke down at $i = 48$. The relative error is about 10^{-12} and 10^{-6}, for $i = 16$ and $i = 32$, respectively, although the condition numbers of G are as large as about 10^9, 10^{16}, 10^{54}, and 10^{96} for $i = 11, 16, 32$, and 47, respectively; see Fig. 2.1.

Thus, the accuracy was high in such a long sequence, that it was easy to conjecture Theorem 3.2, which was eventually proved. As mentioned in §2.1, the l_2 condition number is sometimes a misleading measure of the expected loss of accuracy, and Fig. 2.2 shows that it drastically changes with the scaling of the ω-axis by some power of 2, although the computation of the recursion coefficients is practically the same.

By the remark at the end of §2.2, the polynomial $\bar{\phi}_j(u) = 2^j \phi_j(u/2)$ satisfies the recurrence relation $\bar{\phi}_j(u) = u\bar{\phi}_{j-1}(u) - (j-1)^2 \bar{\phi}_{j-2}(u)$. In other words,

$\phi_j(t) = 2^{-j}\bar{\phi}(2t)$. Similarly, $\widehat{\phi}_j(t) = \bar{\phi}(2t)\sqrt{2}/j!$.

The expansion of $\bar{\phi}_j(u)$ into powers of u has integer coefficients, which are given for $j \leq 10$, separately for even and odd degree, in the columns of the following tables. The leading coefficients are in the main diagonals.

j:	0	2	4	6	8	10
power:						
0	1	−1	9	−225	11025	−893025
2		1	−14	439	−24940	2250621
4			1	−55	4214	−463490
6				1	−140	21378
8					1	−285
10						1

j:	1	3	5	7	9
power:					
1	1	−5	89	−3429	230481
3		1	−30	1519	−122156
5			1	−91	10038
7				1	−204
9					1

For example, the monic orthogonal polynomial

$$\phi_4(t) = 2^{-4}\bar{\phi}_4(2t) = 2^{-4}(9 - 14(2t)^2 + (2t)^4) = \frac{9}{16} - \frac{14}{4}t^2 + t^4.$$

Similarly,

$$\phi_3(t) = 2^{-3}(-5(2t) + (2t)^3) = -\frac{5}{4}t + t^3.$$

A different explicit formula, due to L. Carlitz [3, 1959], is quoted in §5.1.

We now proceed to the nodes $\omega_{n,j}$ and weights $q_{n,j}$ for the Gauss-Lindelöf rules. These are independent of m. We follow the notations of §2.4, except that t is replaced by ω. Set $g_j = g^L_{m^*}(\omega_j)$. For $j > 0$, ω_j equals one of the positive nodes λ_k, and $q_{n,j} = 2d_k^2$. For $j = 0$, $\omega_0 = 0$, and the factor 2 is to be omitted for $q_{n,0}$. By (2.45), the Gauss-Lindelöf rule then reads

$$\int g^L_{m^*}(\omega)w^L(\omega)\,d\omega \approx \begin{cases} \sum_{j=1}^{n/2} q_{n,j}g_j, & \text{if } n \text{ is even;} \\ q_{n,0}g_0 + \sum_{j=1}^{(n-1)/2} q_{n,j}g_j, & \text{if } n \text{ is odd.} \end{cases}$$

The nodes $\omega_{n,j}$ are the singular values of the matrix B,

$$B = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & \dots \\ 2 & 3 & 0 & \dots \\ 0 & 4 & 5 & \dots \\ 0 & 0 & 6 & \dots \end{pmatrix}.$$

When the weights were computed by means of the first components of the singular vectors, according to §2.4, the relative accuracy became very poor for small weights, with the available software (of good reputation). See Fig. 2.4.

A more "robust" computation of the weights is used instead. In order to simplify the correspondence with the theory in §2.3, we describe it in terms of the tridiagonal matrix J (instead of the bidiagonal matrix B). After the computation of the nodes, we compute the matrix $\widehat{\Phi}$ by the forward use of the three term recurrence relation. The equation $V = \widehat{\Phi}D$, see (2.23), then shows that the elementwise division of V by $\widehat{\Phi}$ provides, in the kth column, n values for d_k, which are more or less sensitive to the influence of rounding errors. Let these n values be rearranged according to magnitude. Then compute the $n-4$ averages of 5 successive values. The final estimate is the average of the two estimates which are closest to each other. (We omit the description of the case $n \leq 5$, and the handling of some tie situations, that never occurred in our practice.) The writer also tried the median. It worked well in Example 3.3 below, but the theoretical support is weak, with the incomplete knowledge about the error propagation in this problem.

It is possible that this procedure will not be needed in the future, since Professor C. Moler's more elegant suggestion, mentioned in §2.4, may prove to be satisfactory in more general situations. The suggestion is "to literally rotate the matrix B 180°" so that B becomes

$$\bar{B} = \frac{1}{2}\begin{pmatrix} n-1 & n-2 & 0 & \dots \\ 0 & n-3 & n-4 & \dots \\ 0 & 0 & n-5 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

In the Golub-Welsch formula the relevant vector is then the *last* row of the left factor of the SVD. So far it has helped in practice. The relative difference between the weights obtained in this way and the "robust weights" never exceeds 2000 `macheps` for $n \leq 60$.

If the *eigenvectors* of J (without a "rotation") are used in the Golub-Welsch formula (2.34), instead of the singular vectors of B, the weights are obtained with comparable accuracy. The nodes and weights were computed for $n \leq 64$, by means of the exact recursion coefficients. A few of these results are reproduced here. Note that, for each n, the sum of the weights equals $\mu_0 = \frac{1}{2}$.

These tables indicate that for $4 \leq n \leq 30$, $n - \sqrt{n}$ and $1/(2\sqrt{\log n})$ are crude approximations to the largest and the smallest nodes, respectively. It is not claimed that these formulas are asymptotically correct.

nodes $n=2$	weights	nodes $n=3$	weights
0.5	0.5	1.118033988749895	0.1
		0	0.4

nodes $n=4$	weights	nodes $n=5$	weights
1.825140769936442	1.282917548737155E-2	2.581758305384656	1.336242484891108E-3
.4109272075633473	4.871708245126284E-1	.9135228801608363	1.391131957173561E-1
		0	3.595505617977529E-1

nodes $n = 6$	weights	nodes $n = 7$	weights
3.370828693386971	1.223407724290348E-4	4.183291543696620	1.023405065729494E-5
1.500000000000000	2.597402597402594E-2	2.140529970514226	3.887491425770930E-3
.3708286933869707	4.739036332535445E-1	.8174370347413366	1.601442692742280E-1
		0	3.359580052493438E-1

nodes $n = 8$	weights	nodes $n = 10$	weights
5.013590998533394	8.001981823412229E-7	6.713998580578509	4.218621455080911E-9
2.819460883146335	5.028132602853774E-4	4.259481576640110	6.225131684773411E-6
1.339565281839086	3.642548641342816E-2	2.526738310307730	1.061793131887495E-3
.3465695940557425	4.630709001281033E-1	1.239309786252533	4.474097721942072E-2
		.3297643449118767	4.541910002983865E-1

nodes $n = 12$	weights	nodes $n = 14$	weights
8.453347903173963	1.92837958162765E-11	10.22108146406223	7.95592305804367E-14
5.777514103673806	5.832275927573558E-8	7.351118932789519	4.49706641736970E-10
3.838414271325175	1.963104592549384E-5	5.234967120496440	2.692429594544697E-7
2.336827448313167	1.717789945684028E-3	3.557141316039247	4.219281804600763E-5
1.168953990294477	5.150927695826492E-2	2.200580917974644	2.419066880760435E-3
.3171749309554650	4.467532437080832E-1	1.115997338946113	5.714388502817652E-2
		.3072500755830933	4.403945855802724E-1

nodes $n = 16$	weights	nodes $n = 18$	weights
12.01058333490213	3.03663974943886E-16	13.81740174777518	1.08999946639983E-18
8.966709918439545	2.99837271048565E-12	10.61534348358555	1.78479281618689E-14
6.694226574496088	2.973809336675933E-9	8.202138454558078	2.78216796779075E-11
4.864120937429322	7.656859607867542E-7	6.236840447479230	1.109251804680936E-8
3.351505108292601	7.366601092222453E-5	4.588698971769358	1.661762357359788E-6
2.096580573878714	3.135307274955956E-3	3.192487340453952	1.131623459449303E-4
1.074215034819995	6.192609712010618E-2	2.013754644146923	3.849097691308150E-3
.2991399916273569	4.348641609312475E-1	1.040113898109668	6.605069861460117E-2
		.2923342448020694	4.299853684654316E-1

nodes $n = 20$	weights	nodes $n = 30$	weights
15.63838144144657	3.72211065232145E-21	24.89059235467940	1.03374776317862E-33
12.29077851842402	9.69621421543740E-17	20.94348405071561	1.80927133069462E-28
9.749119413395031	2.28051839578041E-13	17.88034959027363	2.23920787957928E-24
7.661613553430950	1.34725258658107E-10	15.30477809470250	6.28352455045472E-21
5.892640787977603	2.985266996023355E-8	13.06298951129011	6.33046362253946E-18
4.373283447600949	3.042283435423722E-6	11.07505770742079	2.91299311560182E-15
3.064661226519408	1.595900136242516E-4	9.293018844648667	7.07728697852114E-13
1.945718906956708	4.550576509929410E-3	7.685623687341179	9.97731346586592E-11
1.011562470306445	6.965620066409162E-2	6.231567882358909	8.700920021927225E-9
.2865048435249019	4.256305605412983E-1	4.916142168252414	4.902084626834046E-7
		3.729554787153382	1.834079202366247E-5
		2.666322121641025	4.614669064534812E-4
		1.725830933638742	7.756170389583585E-3
		.9160218796471180	8.268757873358269E-2
		.2661052306485067	4.090759441684911E-1

3.5 Numerical studies with Lindelöf's formula.

The tables of the following examples contain *the relative errors divided by* `macheps` $= 2^{-53} = 1.1 \cdot 10^{-16}$.

As explained in the introduction, the "head" of the series, i.e., the first $m - 1$ terms are added, while the convergence acceleration, i.e., the Lindelöf summation formula with a Gauss-Lindelöf rule applied to the integral, is applied to the "tail" of the series.

In each row m is constant. In each column the number of nodes, n, in the Gauss-Lindelöf rule is constant. The value of n is given at the top of the column; due to the symmetry, the number of terms in the rule is $\frac{1}{2}n$.

For example, in the first table, an item of the second row, i.e., $m = 6$, reads $4E6$. It is located in the column, where you read $n = 8$ on the top. Hence, in the application to the series $\sum_{k=1}^{\infty}(-1)^{k-1}1/k$ with $m = 6$, $n = 8$ the relative error is $4{\cdot}10^{6}$ `macheps`. The actual relative error is therefore about $4{\cdot}10^{-10}$.

The exponential part is omitted when when it should have been E0. This makes it easy to find the places where "full accuracy" has been reached.

EXAMPLE 3.1. *Convergence acceleration of four alternating series. Errors with* `macheps` *as unit;*

$$\text{sum} = \sum_{k=1}^{\infty}(-1)^{k-1}f(k).$$

We see in Tables A–D below that the error depends on (m, n) in almost the same way in all four cases, even though $f(k)$ behaves rather differently for large k. We also see that above the main diagonal of a table it is more profitable to increase m than to increase n; below the diagonal it is the other way around. Moreover, it is seen that along the main diagonal the error is divided by approximately 1000, when both m and n are increased by 2. Full accuracy is obtained when $m = 12$, $n = 10$. This happened also when the nodes and weights had been computed by means of the power basis; it was mentioned above that the recursion coefficients became exact for $n \leq 11$.

The convergence as $n \to \infty$ for m fixed is very slow. In case A, which shows the effect of a simple pole at the origin, it was experimentally found that the error is approximately

$$-\frac{1}{2n} + \frac{1}{4n^2} - \frac{1}{8n^4} + \frac{1}{4n^6} - \frac{1}{n^8} \quad \text{for} \quad m = 1,\ n = 20 : 2 : 60.$$

Case B has also a simple pole at the origin with the same residue as case A. Case A, with the known sum $\log 2$, can therefore, as suggested in Chapter 1, be used as a *comparison series.* i.e. one makes a correction of the value obtained, for a certain (m, n) in case B by means of the actual error obtained for the same (m, n) in case A.

A. $f(s) = \dfrac{1}{s}$, $\text{sum} = \log 2 = 0.6931471805599453$.

$n =$	2	4	6	8	10	12
$m =$						
4	2E12	7E10	6E9	1E9	2E8	7E7
6	3E11	2E09	6E7	4E6	4E5	6E4
8	6E10	1E08	2E6	5E4	3E3	2E2
10	2E10	2E07	1E5	1E3	4E1	2
12	8E09	4E06	9E3	8E1	2	2
14	4E09	9E05	1E3	8	2	2
16	2E09	3E05	2E2	2	2	2

B. $f(s) = \dfrac{1}{\log(s+1)}$, sum = 0.9242998972229387.

$n =$	2	4	6	8	10	12
$m =$						
4	2E12	5E10	5E9	8E8	2E8	5E7
6	2E11	2E09	4E7	3E6	3E5	5E4
8	5E10	1E08	1E6	4E4	2E3	2E2
10	2E10	2E07	8E4	1E3	3E1	4
12	7E09	3E06	7E3	6E1	2	2
14	3E09	7E05	1E3	6	2	2
16	2E09	2E05	2E2	2	2	2

C. $f(s) = \exp(-\sqrt{s})$, sum = 0.2256921834909404.

$n =$	2	4	6	8	10	12
$m =$						
4	2E12	2E10	1E9	2E8	3E7	8E6
6	3E11	9E08	2E7	8E5	8E4	1E4
8	8E10	1E08	7E5	1E4	6E2	5E1
10	3E10	2E07	5E4	6E2	1E1	2
12	1E10	4E06	6E3	4E1	0	2
14	7E09	1E06	1E3	4	0	2
16	4E09	4E05	2E2	0	0	0

D. $f(s) = \dfrac{1}{s^2+1}$, sum = 0.3639854725089334.

$n =$	2	4	6	8	10
$m =$					
4	4E12	9E10	4E9	−1E8	−2E8
6	4E11	3E09	9E7	4E6	2E5
8	7E10	2E08	3E6	8E4	3E3
10	2E10	3E07	2E5	3E3	7E1
12	6E09	5E06	2E4	1E2	2
14	2E09	1E06	2E3	1E1	−1
16	1E09	3E05	3E2	0	−1

We shall now see how the technique with a comparison series works for a few values of (m, n). The second and third items are `error/macheps` for case B *without* and *with* the use of case A as a comparison series, respectively.

m	n	Without comparison	With comparison
1	10	5E14	1E10
1	30	2E14	5E8
4	10	1E8	3E4
4	30	2E5	3

In the four cases A–D, $f(s)$ is analytic and bounded for $\Re s \geq \sigma_0 > 0$; there exists an absolutely convergent Laplace-Stieltjes integral representation, see §3.7:

$$f(s) = f_1(s) = \int_0^\infty e^{-sx}\, d\alpha(x), \tag{3.24}$$

where α is a usually unknown function of bounded variation. Eq. (3.24) defines a class of functions that is important per se, and can be used for the analysis of many numerical methods.

If $\alpha(x)$ is non-decreasing, we have a *completely monotonic function.* The term *c.m.* will be used for this, both as an adjective and as a noun in singular and plural. We shall use the terminology and some properties of these which are discussed in an appendix labeled §3.7. A function that satisfies (3.24) is thus a difference of two c.m. The reader who is not familiar with these notions is advised to read §3.7 first.

There is at least one singular point on the imaginary axis in these examples. It is then practical to choose σ_0 a little away from the imaginary axis, $\sigma_0 = \frac{1}{2}$ (say), so that $\int_0^\infty e^{-\sigma_0 x}\, |d\alpha(x)|$ is of moderate size.

We saw that the technique with a comparison series worked well in an example, but it is not really necessary for series of this type, because there is no disadvantage increasing m instead. We shall see other types of series below, where the use of a comparison series is more important, Example Li4, and §3.6.

The following rule of thumb is obtained from Fig. 3.4, which is based on a theory given in Example 3.2:

$$n = \frac{|\log_{10} \mathrm{tol}|}{1.6}, \quad m - \sigma_0 - n = \begin{cases} 2, & \text{if } 2 \leq n \leq 12; \\ 4, & \text{if } 14 \leq n \leq 24, \end{cases} \tag{3.25}$$

where tol is the tolerated error, relative to the size of a term, where the series begins to become slowly convergent. As a check one can make another computation, where m and n are decreased by 2. The result of the first computation is accepted if the difference of the results does not exceed 1000 times the acceptable error; if it does, a new computation is suggested with larger values of m and n.

In the cases A, B, C $\alpha(x)$ is non-decreasing for $x \geq 0$. In other words, the function $f(s)$ and the sequence $\{f(k)\}$ are completely monotonic. In case D, we can only claim that $\alpha(x)$ is of bounded variation, i.e. that $f(s)$ is the difference between two completely monotonic functions. In fact

$$\frac{1}{s^2+1} = \frac{1}{s^2-1} - \frac{2}{s^4-1}.$$

We note that all errors have the same sign in the cases A, B, C, while in case D there are sign changes in the table. (Note that m and n are even.) It is natural to ask whether the error is always positive when $f(s)$ is completely monotonic. It is, by (3.24), with $\alpha(x)$ non-decreasing, sufficient to study $f(s;x) = e^{-sx}$. This will be done in Example 3.2. Although the theoretical answer is "no", the practical answer is "yes", if the above recommendations concerning the choice of

m, n are followed, since the contributions from values of x with negative errors are likely to be much smaller than the tolerance.

The trapezoidal rule with a fixed step size $\Delta\omega$ is a natural alternative to a Gauss-Lindelöf rule for an integrand that decays rapidly as $|\omega| \to \infty$. Is exponential decay fast enough? The error has then two components: the error of the infinite trapezoidal sum and the error due to the truncation to a finite sum. We make a heuristic study for the case $g_{m^*}^L(\omega) \equiv 1$, as a guide for experiments with the four series above.

The first component can be estimated by means of the first terms of Poisson's summation formula, see Fettis [6, 1955]. By (3.3), the Fourier transform of the density function is $\widehat{w}^L(t) = 1/(2\cosh(t/2))$. The estimate becomes $2\widehat{w}^L(2\pi/\Delta\omega) = 1/\cosh(\pi/\Delta\omega)$.

In the second component, set $\Omega = \max \omega$. If the tolerated error is small enough, we have $\cosh(\pi\omega) \approx \frac{1}{2}\exp(|\pi\omega|)$ for $|\omega| \geq \Omega$. We also approximate the neglected tail of the trapezoidal sum by the integral

$$\int_{|\omega|\geq\Omega} w^L(\omega)\, d\omega \approx 1/(\pi \cosh \pi\Omega).$$

It is almost optimal to choose the two components almost equally small. If we choose $1/\Delta\omega = \Omega = -\pi^{-1}\log\epsilon$, the error estimate becomes $(2 + 2/\pi)\epsilon$, and the number of complex function evaluations becomes $N = \Omega/\Delta\omega + 1 \approx \Omega^2 = \pi^{-2}|\log\epsilon|^2 = 0.54|\log_{10}\epsilon|^2$. If $\epsilon = 2^{-53}$, which corresponds to "full accuracy", we obtain $N \approx 137, \Omega = 11.7, \Delta\omega = 0.086$, and the error estimate becomes $3{\cdot}10^{-16}$.

The writer made computations with the series A–D with $N = 129, \Omega = 11$, hence $\Delta\omega = 0.086$, and obtained almost "full accuracy" in these four cases. With the Gauss-Lindelöf we had almost "full accuracy" for $n = 10$, $m = 12$, i.e. with 5 complex function evaluations and 12 real function evaluations. We can therefore claim that *the trapezoidal rule requires more than 10 times as much work for "full accuracy" for a slowly convergent alternating series*, at least when $f(s)$ is completely monotonic, or is the difference of two completely monotonic functions. More generally, the above heuristic theory implies that *the amount of work for the trapezoidal rule is proportional to* $|\log\epsilon|^2$, *while it is only proportional to* $|\log\epsilon|$ *for the Gauss-Lindelöf rule*, by (3.25).

We must point out that there are many convergent alternating series that cannot be handled by the Lindelöf formula. One example is the series generated by $f(s) = \exp(-as^2)$, $a > 0$, $s = \sigma + i\omega$ because, for $\sigma = m - 1/2$, $|\exp(-as^2)| = \exp(a\omega^2 - a\sigma^2)$ does not satisfy the assumptions (b) and (c) made in §3.1. The Lindelöf summation cannot be used, nor is it needed, unless $a \ll 1$. The Poisson summation formula is recommended instead for series of this type.

Another interesting class of series is generated by $f(s) = f_1(s)/\Gamma(as)$, $a > 0$, where $|f_1(s)| \leq C_1$ for $\Re s \geq \sigma_0$. For $\sigma \geq \sigma_0$ fixed, and $|\omega| \gg 1$, we have by Stirling's formula,

$$|f(\sigma + i\omega)| = C(a\sigma)|\omega|^{-a\sigma+1/2}e^{a|\omega|\pi/2}(1 + o(1)). \tag{3.26}$$

The Lindelöf formula can thus be used for $a \leq 2$ only. A more rapid decay of the terms of the original series makes the performance of the Lindelöf formula worse. We shall return to this example, multiplied by $(\pm z)^s$, in §3.6 and §4.6.

Similar remarks are relevant for all our four summation formulas, except that, for the Plana and the Midpoint formulas, the condition in the second case becomes $a \leq 4$ due to the more rapid decay of $w^P(\omega)$ and $w^M(\omega)$.

EXAMPLE 3.2. $f(s;x) = e^{-sx}$, $x > 0$; *with extension to alternating series that satisfy* (3.24).

This is a theoretical study of the application of the Gauss-Lindelöf rule on a class of series, exemplified in Example 3.1. We shall use the notations of §2.3, except that the independent variable is now ω instead of t; x is to be considered as a positive parameter; $w^L(\omega) = 1/(2\cosh \pi\omega)$. Integrals without limits are over $\mathbf{R}$. *We confine the discussion to even values of* m *and* n. If needed, the results can be easily modified to odd values.

The sum of the alternating series is in this case $-(e^x+1)^{-1}$, and the tail equals $-e^{(1-m)x}(e^x+1)^{-1}$. By (3.1), the tail equals the integral

$$\int e^{(-m^*-i\omega)x} w^L(\omega)\, d\omega = \int g^L(\omega;x) w^L(\omega)\, d\omega, \text{ where } g^L(\omega;x) = e^{-m^*x}\cos\,\omega x.$$

(Recall that $m^* = m - \frac{1}{2}$.) The truncation error of the evaluation of the tail by the Gauss-Lindelöf rule with $\frac{1}{2}n$ positive nodes reads $R_n g^L(\cdot;x)$, see Fig. 3.3.

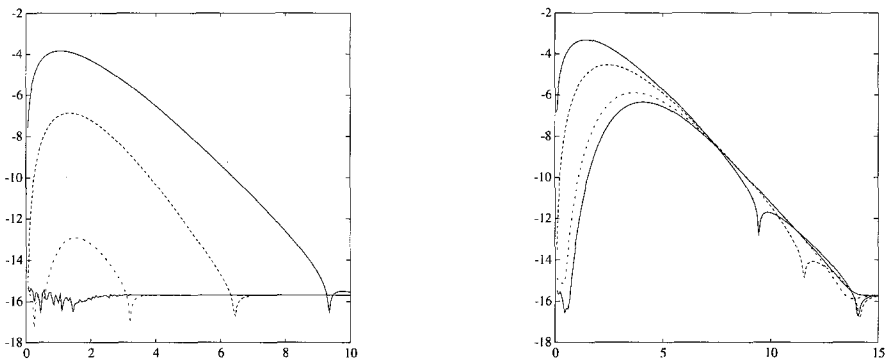

Figure 3.3: $\log_{10}|R_n g^L(\cdot;x)|$ for $n = 2:2:10$. To the left: $f(s) = e^{-xs}$, $m = n+2$; To the right: $f(s) = e^{-xs}$, $m = 3$. All curves are computed as the difference between Gauss-Lindelöf results and exact results, without the use of (3.28).

We first note that $|R_n g^L(\cdot;x)| \leq e^{-m^*x}$, by (2.33), with $\alpha = 1$, $P = 0$. This is no good for small values of x. So, as in §2.3, let $P \in \mathcal{P}_{2n}$ be the Hermite interpolation polynomial determined by the conditions, $P(\lambda_k) = g^L(\lambda_k;x)$; $P'(\lambda_k) = g'_L(\lambda_k;x)$, $k = 1:n$. By (2.29),

$$(3.27)\quad g(\omega) - P(\omega) = r_n g_L^{(2n)}(\xi_\omega;x)\widehat{\phi}_n(\omega)^2 = r_n e^{-m^*x} x^{2n} \cos\,\xi_\omega x \widehat{\phi}_n(\omega)^2.$$

Hence, by (2.27), together with the bound $|R_n g^L(\cdot;x)| \le e^{-m^* x}$ given above, we obtain

$$|R_n g^L(\cdot;x)| \le e^{-m^* x} \min\{r_n x^{2n}, 1\}. \tag{3.28}$$

For the application to a series, where $f(s) = f_1(s)$ satisfies (3.24). the truncation error becomes

$$T_{m,n} f = \int_0^\infty R_n g^L(\cdot;x)\, d\alpha(x),$$

hence $|T_{m,n} f| \le M_{m,n} \int_0^\infty e^{-\sigma_0 x} |\, d\alpha(x)|$, where we set $\bar{m} = m - \frac{1}{2} - \sigma_0$,

$$M_{m,n} \equiv \max_{x>0} e^{-\bar{m}x} \min\{r_n x^{2n}, 1\} \approx \tilde{M}_{m,n} \tag{3.29}$$

$$\tilde{M}_{m,n} \equiv \max_{x>0} e^{-\bar{m}x} \min\left\{ x^{2n} 2^{-4n} \sqrt{\frac{n\pi}{4}}, 1 \right\}. \tag{3.30}$$

(We used (3.23) here.) The number of correct decimal digits is measured by $\log_{10} \tilde{M}_{m,n} \approx \log_{10} M_{m.n}$, while the computational work is measured by $k = \bar{m} + n$. (Both measures are open to criticism.)

We first estimate $\tilde{M}_{m,n}$. Note that $e^{-\bar{m}x} x^{2n}$ has a local maximum equal to $e^{-2n} \bar{x}^{2n}$ when $x = \bar{x} \equiv 2n/\bar{m}$; we call $\bar{x}$ *"the worst x"*. Hence

$$\log \tilde{M}_{m,n} = 2n(\log \bar{x} - 1 - 2\log 2) + \frac{1}{2} \log(n\pi/4)$$

if $2n \log(\bar{x}/4) + \frac{1}{2} \log(n\pi/4) < 0$. (This condition is satisfied in all interesting cases.)

Next we compute the value of $2n/\bar{m} = \bar{x}$ that minimizes $\tilde{M}_{m,n}$, for a given amount of "work" $k = \bar{m} + n$. Note that $n = k\bar{x}/(2 + \bar{x})$. By straightforward calculation, we find that $\log \tilde{M}_{m,n}$ is minimal when

$$\log \bar{x} + \frac{\bar{x}}{2} - 2\log 2 + \frac{2 + \bar{x}}{4k\bar{x}} = 0; \quad \text{i.e.,} \quad \bar{x} \approx 1.705 - \frac{1}{2k}. \tag{3.31}$$

(The error of the approximation is less than 0.001 if $k \ge 10$.) As $k \to \infty$, $\bar{m}/n \to 2/\bar{x} = 1.173$, so the optimal path in the (m,n)-table deviates a little from the main diagonal, but that is relevant only if one wants extremely high accuracy. It follows that $\min \log \tilde{M}_{m,n} = -\bar{x}k + \frac{1}{2} \log k - 1.013 \pm 0.004$ for $k \ge 10$.

Fig. 3.4 was constructed by means of these equations together with the formulas $n = k\bar{x}/(2 + \bar{x})$, $\bar{m} = k - n$, $m = \bar{m} + \frac{1}{2} + \sigma_0$.

Measuring work by the parameter k means that the evaluation of $f(s)$ for a real s costs 1 unit, while the evaluation of $\Re f(s)$ for a non-real s costs 2 units. The formula for $\min \log M_{m,n}$ implies that, for large k, one unit of work yields $\bar{x}/\log 10 = 0.741$ decimal digits, hence "full accuracy" costs 22 units of work, in excellent agreement with Example 3.1.

This can be compared with the results of Dahlquist, Gustafson and Siklósi [5, 1965, § 4], that the Euler transformation, with optimal division of a sequence into a head and a tail, yields $\log_{10} 3 = 0.477$ decimal digits for one unit of work, while a kind of Chebyshev acceleration, later algorithmically modified and improved

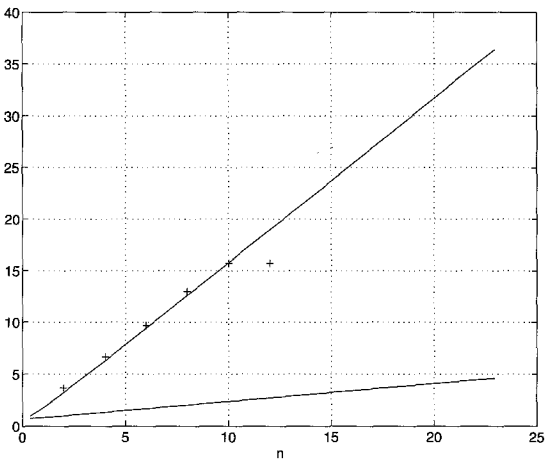

Figure 3.4: The number of correct decimal digits in the sum versus n with optimal m for "the worst x", when $f(s;x) = e^{-sx}$. The lower curve shows the optimal choice of $\bar{m} - n$. The + points are results from Example 3.1, case A, $m = n + 2$.

by Gustafson [7, 1978], yields $\log_{10}(3 + \sqrt{8}) = 0.766$ decimal digits for one unit of work, hence Gustafson's Chebyshev acceleration is about 3 % more efficient than the Gauss-Lindelöf rule.

The cost for "full accuracy" is for the three methods mentioned thus 22, 34 and 21 units of work, respectively. It has been experimentally found that the ϵ-algorithm and Gustafson's Chebyshev acceleration both need on the average 20 terms for full accuracy.

We are also interested in the sign of the remainder. The cusps in the right part of Fig. 3.3 indicate that there are sign changes of $R_n g^L(\cdot;x)$. Probably, $R_n g^L(\cdot;x) > 0$ to the left of the first visible cusp of each curve, but since there may be some doubts, whether the irregularities near the origin are entirely due to rounding errors, we make a study for small values of x. By (3.27),

$$R_n g^L(\cdot;x) = \int (g^L(\omega;x) - P(\omega))w^L(\omega)\,d\omega = r_n e^{-\bar{m}x} x^{2n}(a_1 + a_2),$$

where

$$a_1 = \int_{|\omega|<\Omega} \cos\omega x\ \widehat{\phi}_n(\omega)^2 w^L(\omega)\,d\omega, \quad a_2 = \int_{|\omega|>\Omega} \cos\omega x\ \widehat{\phi}_n(\omega)^2 w^L(\omega)\,d\omega.$$

Choose $\Omega = \pi/(3x)$, and set $\eta = \int_{|\omega|>\Omega} \widehat{\phi}_n(\omega)^2 w^L(\omega)\,d\omega$. Then $a_1 + a_2 > \frac{1}{2}(1-\eta) - \eta > 0$ if $\eta < 1/3$. Supported by Fig. 3.3, we conjecture that $\eta < 1/3$ if $\Omega \geq n$, i.e., if $x \leq \pi/(3n)$. We conclude that

$$R_n g^L(\cdot;x) > 0 \quad \text{if } x \leq \pi/(3n). \tag{3.32}$$

EXAMPLE 3.3. *Power series and Fourier series.*

In order to apply the Lindelöf formula to a power series, we introduce one more complex variable $z = |z|e^{i\psi}$. Let δ be any positive number. Set, for $|\pi - \psi| \leq \pi - \delta$,

$$(-z)^s = |z|^\sigma e^{\omega(\pi-\psi)} e^{i(\omega \log|z| - \sigma(\pi-\psi)}. \tag{3.33}$$

Put $f(s) = f(s;z) = (-z)^s f_1(s)$ into (3.21), where $f_1(s)$ satisfies (3.24), and set

$$F(z) \equiv \sum_{k=1}^{\infty} f_1(k) z^k \tag{3.34}$$

$$F(z) = \sum_{k=1}^{m-1} f_1(k) z^k + (-1)^{m-1} \int g^L_{m^*}(\omega; z) w^L(\omega)\, d\omega. \tag{3.35}$$

(Recall that $m^* = m - 1/2$.) Eq. (3.34) defines an analytic function in a circle $|z| \leq r$. We know that $r \geq 1$, since $\{f_1(k)\}$ is bounded. On the other hand, (3.35) defines an analytic function in the z-plane, cut along the positive real axis, because the integrand is, for any $R > 0$, $\delta > 0$, majorized by $R^{m^*} e^{-\delta|\omega|}$ in the region defined by the inequalities $|z| \leq R$, $|\pi - \psi| \leq \pi - \delta$.

These functions coincide in the intersection of their regions of validity; a fact that has been anticipated in the notation. Eq. (3.35) therefore provides an analytic continuation to the union of these regions, i.e., to the z-plane, cut from r to ∞ along the real axis. The question is: how well can this be approximated by means of Gauss-Lindelöf rules?

Note that the assumptions for the derivation of Lindelöf's summation are relevant for obtaining a start for the process of analytic continuation only. They are irrelevant, after analytic continuation has been applied. For example, assumption (c) of §3.1 is no longer valid when $|z| > r$. Anyway, the analytic continuation requires the convergence of the Lindelöf integral, so at least the restrictions on the growth of $f(m^* + i\omega)$, $|\omega| \to \infty$ cannot be ignored.

In *this* example we consider Fourier series, which can be computed by means of $F(z)$ for $z = e^{i\psi}$, $0 < \psi \leq \pi$; more specifically the case where $f_1(s) = s^{-1}$. The sum equals $F(z) = -\log(1-z) = -\log 2\sin\frac{\psi}{2} - \frac{i(\pi-\psi)}{2}$. Note that for $\psi = 0$ we have a divergent series with positive terms, while for $\psi = \pi$, the series is the alternating series Example 3.1, case A (with sign reversed).

There are two sources of possible trouble:

- The decay of the integrand is only like $e^{|\pi-\psi||\omega|} w^L(\omega)/|m^* + i\omega| = e^{-|\psi\omega|}/|m^* + i\omega|$.
- There is a pole of $f_1(s)$ at the origin.

The nearness to the pole may be the dominant error source for (say) $\psi \geq \frac{\pi}{2}$. We could use the comparison series $\sum (-1)^k k^{-1}$ here, but it seems easier to escape from the pole by increasing m in this example just like in Example 3.1. For smaller values of ψ the slow decay of the integrand takes over the role as the

dominant error source, and the writer does not know how to cure that efficiently by a comparison series.

The largest node is a little less than n. In order to obtain d significant decimal digits, it is thus conceivable that $e^{-|\psi n|}$ should not be much larger than 10^{-d}, i.e., n should be something like $2.3d/\psi$. Actually, the results below indicate that this is a little larger than necessary.

Computations were made with several values of m and n, $n \leq 64$. The best errors $\epsilon_{m,n}$ obtained are tabulated below. We there exclude some "occasional good results" obtained for lower values of n, where the error changed sign, since such a result would not have been recognized in a realistic example, where the exact sum is not known. "Convergence ratio" means the ratio $\epsilon_{m,n}/\epsilon_{m-2,n-2}$ or, for $\psi < \frac{1}{2}\pi$, $\epsilon_{m,n}/\epsilon_{m,n-2}$, estimated by experiment.

ψ	π	$3\pi/4$	$\pi/2$	$\pi/4$	$\pi/8$	$\pi/16$	$\pi/64$	$\pi/256$
`error/macheps`	1	1	1	1	$6E3$	$2E9$	$3E13$	$6E14$
$m;n$	12; 10	12; 10	8; 16	6; 42	4; 64	2; 64	2; 64	2; 64
convergence ratio	0.001	0.001	0.03	0.20	0.44	0.66	0.88	0.96

The primary output (not displayed here) shows that the convergence ratio is amazingly independent of n, until the error is at the level of rounding errors. This indicates that further improvement can be obtained by the use of higher values of n, or by Aitken extrapolation. (In the writer's experiments n was limited by certain software restrictions on the size of a matrix.)

A preliminary experiment was made with *Aitken extrapolations* of the Gauss-Lindelöf results obtained with $n = 52 : 2 : 60$ for $\psi = \pi/8$, $\pi/16$, $\pi/64$. It proved so successful that Aitken extrapolation was applied also to the extrapolated sequences, and this was also successful. For $\psi = \pi/16$ the improvement was about 4 decimal places for the two extrapolations together.

As in the previous tables, the relative errors are divided by `macheps`.

ψ	$\pi/8$	$\pi/16$	$\pi/64$
Orig. error, $n = 60$	$2E4$	$6E9$	$4E13$
Aitken extrapol.	$5E1$	$3E7$	$2E12$
Iterated Aitken	-7	$5E5$	$2E11$
$m;n$	4; 60	4; 60	2; 60

It would have been more economical to apply the extrapolation to the sequence obtained with a sparser sequence of values of n. It is questionable how much efforts like this should be made to improve the Gauss-Lindelöf results.

The Plana formula applied to the same series converges much faster for small values of ψ, see §4.4, Example 4.3. The price paid for the fast convergence of the Plana formula is the computation of $\int_m^\infty z^\sigma f(\sigma; z)\, d\sigma$, and this can sometimes be costly, compared to the few function evaluations requested by the Lindelöf formula. *The writer recommends unconditionally the Lindelöf formula for* $\psi \geq \frac{1}{2}\pi$. Sometimes it can, perhaps together with Aitken extrapolation, compete with the Plana formula even for (say) $\psi = \pi/16$.

The writer believes that this example is representative for series generated by $f(s) = e^{-i\psi s} f_1(s)$, $0 < |\psi| \leq \pi$; $f_1(s)$ satisfies (3.24). The theoretical support for this belief is so far only that for $\psi = \pi$—see Examples 3.1 and 3.2—the behaviour is essentially the same for any function f_1 of this class.

The above tables of results were obtained by the use of "robustly estimated weights", as described above. When ψ is small, the slow decay of the integrand necessitates large values of n. Even the smallest weights should then have a reasonably good relative accuracy. At least they should not be wrong by several orders of magnitude, like some of the weights shown in the right part of Fig. 2.4. Nor would weights determined from the power basis be sufficiently accurate for small values of ψ.

Some additional experiments were made in order to illustrate these matters. The weights shown in the right part of Fig. 2.4 gave full accuracy for $\psi \geq \pi/2$. (The weights have no serious errors for $n \leq 16$.) For $\psi = \pi/4$, however, the best error, $3 \cdot 10^5$ `macheps` $\approx 3 \cdot 10^{-11}$, was obtained for $n = 14$; for $n > 14$ the errors grew. The experience for $\psi = \pi/8$ was similar; the best error was 10^{10} `macheps` (instead of $6 \cdot 10^3$ `macheps` with the robust weights).

EXAMPLE 3.4. *Analytic continuation of $F(z)$ outside the circle of convergence.*

Recall the introduction of the previous example. Consider again (3.35). Suppose that $f_1(s) = s^{-1}$, hence $f(s;z) = s^{-1}(-z)^s$, $F(z) = -\log(1-z)$, but this time z assumes real negative values outside the unit disk. The power series diverges for $|z| > 1$, but the Lindelöf formula (3.35) provides an analytic continuation. The integrand is the real part of $e^{i\omega \log|z|}(m^* + i\omega)^{-1} w^L(\omega)$, multiplied by the outside factor $|z|^{m^*}$. There are three sources of possible trouble:

- When $|z| \gg 1$, $F(z)$ is a relatively small difference of terms of the size $|z|^{m-1}$. The truncation error is multiplied by the factor $|z|^{m^*}$.
- There is a pole of $f_1(s)$ at the origin.
- The nodes of the Gauss-Lindelöf rule remain rather sparse, unless n is extremely large, and may not be able to resolve the oscillating factor $e^{i\omega \log|z|}$, if (say) $\log|z| \gg \pi$.

We must avoid a large value of m^* here, when $|z|$ is large. On the other hand, if m^* is not large, the nearness to a pole of $f_1(s)$ has also a harmful effect on the truncation error. This seems like a market for the use of a comparison series.

Computations were made for several values of m, n, $n \leq 64$, first *without* the use of a comparison series. They were interrupted at a value of n, $n < 64$, if either "full accuracy" had been obtained, or if the absolute value of the error began to grow. The convergence ratio does not make sense here.

Without a comparison series:

$-z$	1	2	5	10	20	50	100
`error/macheps`	≤ 10	≤ 10	74	554	9858	$3E5$	$5E8$
$m;n$	12; 10	5; 24	4; 36	3; 48	3; 54	2; 64	2; 64

Considering how slowly the distance between the successive nodes shrink as n increases, the accuracy is much better than expected, but note that $\log|z|$ is not very large at these computations.

Then a comparison series was used. Note that the residue of $f(s;z)$ at $s=0$ equals 1 for all z. The error for $F(-1) = -\log 2$ was computed for $m = 0:3$, $n = 10:2:60$ and subtracted from the errors of $F(z)$ for the same z as above. The best result was always obtained for $m=1$. Full accuracy was obtained for $-z \leq 20$; for larger values of $-z$ the comparison series technique improved the results by more than 3 digits. In addition to the table below, $F(-500)$ is correct to 5 digits, and $F(-1000)$ is correct to 3 digits. When $|z| \gg 1$, the error decreases rather slowly with n. The improvement in $F(-100)$ from $n=32$ to $n=60$ is 5 digits; for $F(-1000)$ it is less than 2 digits.

With a comparison series:

$-z$	1	2	5	10	20	50	100
error/macheps	–	≤ 10	≤ 10	≤ 10	≤ 10	80	$3E5$
$m;n$	–	1;2	1;34	1;50	1;50	1;56	1;60

3.6 Application to ill-conditioned power series.

We call an infinite series *ill-conditioned if small relative changes of the terms can cause a large change of its sum*, relative to some natural reference for the sum. A typical example was mentioned in Ch. 1. The series converges for all z, but the modulus of the terms increases rapidly at the beginning. The plot of the terms, Fig. 1.1, is reminiscent of an earthquake with an epicentre at $k \approx 2y-1$. Numerically this means catastrophic cancellations, if the sum is evaluated by the addition of terms or by the Horner scheme. The terms behave in the opposite way to the terms of a semi-convergent series. An alternative name to "ill-conditioned" could be "semi-divergent".

EXAMPLE 3.5. *A series related to the exponential integral.* Set

$$(3.36)\quad f(s;z) = \frac{(-z)^s}{s\Gamma(s+1)}, \quad F(z) = \sum_{k=1}^{\infty}(-1)^k f(k;z) = \int_0^z \frac{e^{-t}-1}{t}\,dt.$$

In the notation of Abramowitz and Stegun [1], Ch. 5, $F(z) = -E_1(z) - \log z - \gamma$; γ is Euler's constant. The logarithm is the dominant part when $|z|$ is large.

The term with the largest modulus is obtained for $k \approx |z|-1$. By Stirling's formula, $|f(|z|-1;z)| \sim Ce^{|z|}|z|^{-3/2}$. For $z=-100$, this becomes 10^{40}, while $F(-100) \approx -5$.

The integrand in Lindelöf's integral (including w^L) is, by (3.26) and (3.33),

$$C|z|^{m-1/2}e^{i\omega\log|z|}O(|\omega|^{-m-1}e^{-|\omega|\pi/2}), \quad |\omega| \gg 1.$$

The sources of trouble are of the same kind as in Example 3.4, and the experiences are qualitatively similar.

The table below contains numerical results for these examples. The first two rows are the average absolute errors, for $50 \leq n \leq 60$, with `macheps` as unit, obtained without a comparison series, for $m = 4$ and $m = 5$, respectively.

In the last row the series generated by $f(s) = s^{-1}$ is used as a comparison series. The notation $m = 1\mathrm{C}$ means $m = 1$ with a comparison series. (This has the same pole and residue as $f(s; z)$ has for every z.) As expected, the improvement obtained by the use of a comparison series increases with $|z|$.

The table this time displays the *absolute* errors divided by macheps; the sum increases from about 1 to 5 as z increases from 1 to 100.

$-z$	10	20	50	100	200	500	1000
`error/macheps`, $m = 4$	$2E3$	$2E3$	$1E5$	$2E6$	$4E7$	$2E9$	$1E16$
`error/macheps`, $m = 5$	$1E3$	$1E4$	$8E5$	$4E7$	$1E9$	$7E10$	–
`error/macheps`, $m = 1\mathrm{C}$	$3E1$	$5E1$	$8E1$	$1E2$	$4E2$	$2E3$	$2E9$

The results for $20 \leq n \leq 30$ had only 5–10 times as large errors when $|z| < 100$.

We also used the series generated by $f(s; -10)$ as comparison series. This changed the absolute errors by about 30 `macheps` (which is the error obtained for $z = -10$ by the aid of the other comparison series.)

The Lindelöf method is not equally successful if, for example, $z = iy$, $y > 0$. The integrand (including w^L) is now $C(\sigma)|z|^\sigma O(|\omega|^{-\sigma-3/2})$, by (3.26) and (3.33) for $a = 1$. The Lindelöf integral converges relatively slowly, perhaps too slowly, since the error analysis of §2.3 (with $w(\omega)/w(\alpha\omega)$) indicates that the Gauss-Lindelöf rule may require some exponential decay of the integrand (though this is a sufficient condition only).

In fact, numerical experiments indicate that the use of the comparison series generated by $f(s) = s^{-1}$, $m = 1$, $n = 60$, seems to be the best alternative when $y \geq 50$, but the accuracy is rather low; the relative error of $\Re F(iy)$ grows from $5 \cdot 10^{-4}$ for $y = 50$ to $5 \cdot 10^{-2}$ for $y = 1000$. For $n = 30$ the errors are about 5 times as large. For $y < 50$, the use of higher values of m gave better results than the use of a comparison series. The error decreases rapidly, as y decreases. Full accuracy is obtained for $y \leq 5$.

Note that the series for $\Re F(iy)$ can also be written $\sum (-y^2)^k/(2k(2k)!)$, and hence it can be treated as a real alternating series, with the same mediocre performance.

This form also reminds of the power series for the cosine function and, more interestingly, for the Bessel function

$$J_\nu(2y) = \sum \frac{(-1)^k y^{2k}}{\Gamma(k+1)\Gamma(k+\nu+1)}, \quad y \in \mathbf{R},\ y \gg 1. \tag{3.37}$$

The performance of the Gauss-Lindelöf rule is mediocre also in this case. The Gauss-Plana rule performs much better, due to the faster decrease of $w^P(\omega)$, but the integral $\int_m^\infty z^\sigma f(\sigma; z)\, d\sigma$ that occurs in the Plana formula here requires a special treatment and relatively much work, see §4.6.

3.7 Appendix. Complete monotonicity and related questions.

We shall study the class of functions that can be represented by a Laplace-Stieltjes integral,

$$f(s) = \int_0^\infty e^{-sx}\, d\alpha(x), \tag{3.38}$$

where α is a *usually unknown* function of bounded variation. (Compare (3.24).) This class is a closure of sums of exponentials and is hence convenient for the analysis of numerical methods for the summation of series, see, e.g., Example 3.2 or Dahlquist et al. [5], and for several other numerical problems. A few of their numerous properties are selected here, with their numerical applications in mind.

The class includes many common functions, e.g., all rational functions that are real on the real axis and bounded in a half-plane. You find more examples below and in tables of Laplace transforms. These may be transformed and combined according to rules given below.

We shall be rather short and refer as much as possible to Widder [12, 1941], [13, 1971, Ch. 5] for proofs and more precise information. Unless the integral converges absolutely for all s or for no s, there is a real number σ_a, such that it converges absolutely when $\Re s > \sigma_a$ but not when $\Re s < \sigma_a$. The function $f(s)$ *is analytic and bounded for* $\Re s \geq \sigma_0$ *for every* $\sigma_0 > \sigma_a$, but this is itself not sufficient for the existence of a representation of the type (3.38). If, however, we add the condition that

$$\int_{-\infty}^{\infty} |f(\sigma + i\omega)|\, d\omega < \infty, \quad f(s) \to 0, \quad \text{as } |s| \to \infty,\ \sigma \geq \sigma_0, \tag{3.39}$$

then $f(s)$ *satisfies* (3.38), see Widder [13, 1971, §5.11], and so does every linear combination of such a function with other functions, for which the validity of (3.38) can be proved by other means. (Condition (3.39) is namely not necessary.) In the general case, we cannot be sure that $f(s)$ has a singularity where $\Re s = \sigma_a$.

If $\alpha(x)$ is non-decreasing, $f(s)$ is called a *completely monotonic function (c.m.)* on the open interval $s > \sigma_a$ and on the interval $s \geq \sigma_0$, for any $\sigma_0 > \sigma_a$. The abbreviation c.m. will be used, both as an adjective and as a noun, and both in singular and in plural. If $f(s)$ is a c.m., it has a singularity at $s = \sigma_a$.

A function satisfies (3.38) *with absolute convergence if and only if it is the difference of two c.m.* (We omit the interval of validity, when it is fairly obvious from the context.)

This property can be used to find that a given function is *not* c.m., e.g. $f(s) = 1/(1+s^2)$ is not c.m., since the rightmost singularities are $s = \pm i$, while $s = 0$ is no singularity. This function, however, is the difference of two c.m., since it is analytic and bounded, and satisfies (3.39), for any positive σ_0. We shall see an actual decomposition below.

Another useful criterion for this kind of negative conclusion is that *a c.m. can never decrease faster than an exponential as* $s \to +\infty$ *along the real axis.* (This follows rather directly from the integral representation.) For example, e^{-s^2} and $1/\Gamma(s)$ are not c.m.

An important extension of the class defined by (3.38) is the class defined by $f(s) = (-z)^s f_1(s)$, $0 < \arg z \leq \pi$, where $f_1(s)$ satisfies (3.38). This is fundamental for the application of the Lindelöf formula and many other numerical methods to power series, see Examples 3.3 and 3.4. The restrictions on $f(s)$ for the Lindelöf formula, see [9], §3.1, are still satisfied in this extension.

The facts mentioned so far are rather powerful for finding out whether a given function is completely monotonic or not, but we shall list some other criteria that may often be easier to apply. The deepest criterion is the following classical theorem of Bernstein.

(A) *$f(s)$ is a c.m. if and only if*

$$f(s) \geq 0, \quad (-1)^j f^{(j)}(s) \geq 0, \ j = 1, 2, \ldots, \ s \in [\sigma_0, \infty). \tag{3.40}$$

The "only if" part follows rather directly from the definition, but the proof of the "if" part is difficult, see Widder [13, 1971], §6.6, §6.7. The theorem states that (3.38) and (3.40) are equivalent; it therefore plays no role that Widder uses (3.40) as the definition, while we use (3.38).

As an application it follows directly from (3.40) that the functions s^{-p}, $s > 0$, $p \geq 0$ are c.m.

(B) *A uniformly convergent positive linear combination of c.m. is itself c.m.*

The term "positive linear combination" includes sums with positive coefficients and, more generally, Stieltjes integrals $\int f(s;p)\, d\beta(p)$, where $\beta(p)$ is non-decreasing.

(C) *If $f(s)$ is c.m., and $a \geq 1$, $b \geq 0$, then $g(s) = f(as + b)$ and $(-1)^j f^{(j)}(s)$, are c.m., $j = 1, 2, 3, \ldots$.*

With appropriate changes of σ_0 for f and g this can be extended to, e.g., $a > 0$ or $b < 0$.

(D) *The product of two c.m. is c.m.*

This can evidently be extended to products of any number of factors. Hint to a proof: use the Leibniz rule to show that (3.40) holds.

A function $F(x)$ is called *absolutely monotonic* in an interval, if $F^{(j)}(x) \geq 0, j = 0, 1, 2, \ldots$ there. If F_1, F_2 are absolutely monotonic (in appropriate intervals) it can be shown by induction that $F_1(x) \cdot F_2(x)$ and $F_1(F_2(x))$ are absolutely monotonic.

(E) *If F is absolutely monotonic in the range of the c.m. $f(s)$, then $F(f(s))$ is c.m.*

Hint: Reduce this to the previous statement about the composition of two absolutely monotonic functions.

Example: $F(x) = 1/(1-x)$ is absolutely monotonic for $0 \le x < 1$, and s^{-p}, $p \ge 0$, is completely monotonic for $s \ge 1$. Hence $1/(s^p - 1) = s^{-p}/(1-s^{-p})$ is completely monotonic for $s > 1$. Hence, the decomposition $\frac{1}{s^2+1} = \frac{1}{s^2-1} - \frac{2}{s^4-1}$ tells that $\frac{1}{s^2+1}$ is the difference of two c.m. for $\Re s > 1$, but by a less constructive argument, we know already that this is true even for $\Re s > 0$.

On the other hand, if $f(s), g(s)$ are c.m., then $F(s) = f(g(s))$ is *not* c.m., unless $F(s)$ is a constant; indeed $F'(s) \ge 0$ while complete monotonicity would require $F'(s) \le 0$.

(F) *If $g'(s)$ is c.m., and f is c.m. in the range of g then $F(s) = f(g(s))$ is c.m.*

(Note that the requirement above may necessitate an increase of σ_0. Also note that $g(s)$ itself is not c.m.)

Hint to a proof: show by induction that

$$(-1)^p F^{(p)}(s) = \sum_{j=1}^{p} \psi_{pj}(s)(-1)^j f^{(j)}(g(s)),$$

where $\psi_{pj}(s)$ is c.m.

This criterion, which is not easily found in the literature, can be used to prove that the functions $\frac{1}{\log(s+1)}$ and $e^{-\sqrt{s}}$, used in the examples of §3.5, are c.m. for $\Re s \ge 1$.

It is left to the reader to find out if or how these properties can be modified for the class of functions defined by (3.38).

Up to now we have mentioned completely monotonic *functions* only. We now define a *completely monotonic sequence* as a sequence $\{u_n\}_0^\infty$ that satisfies the difference analog of (3.40),

$$(3.41) \qquad (-1)^j \Delta^j u_n \ge 0, \quad j, n = 0, 1, 2, \ldots, \quad (\Delta^0 u_n \equiv u_n).$$

We use the abbreviation c.m. also for sequences.

Suppose that $u_n = f(a + hn)$, $a \ge 0, h > 0, n = 0, 1, 2, \ldots$. By a fundamental property of finite differences, e.g., Dahlquist and Björck [4, 1974 §7.3.4],

$$(-1)^j \Delta^j u_n = (-h)^j f^{(j)}(\xi_n) \ge 0.$$

It follows that

(G) *If the function f is c.m., then the sequence $\{u_n\}_0^\infty$ is c.m.*

Conversely, there exists a function $f(s)$ completely monotonic in $[0, \infty)$ that interpolates a sequence $\{u_n\}_0^\infty$, i.e. $f(n) = u_n$, $n = 0, 1, 2, \ldots$, if the sequence is a minimal completely monotonic sequence.

"Minimal" means that the sequence ceases to be a c.m. when u_0 is decreased. (See Widder [12, 1941], §IV.14.) The following theorem of Haus-

dorff, which is analogous to Bernstein's theorem, see Widder [13, §6.6], has also been used in the analysis of convergence acceleration, Dahlquist et al. [5].

(H) *A sequence* $\{u_n\}$ *can be represented as a moment sequence on the interval* $[0,1]$, *i.e.* $u_n = \int_0^1 x^n \, d\beta(x)$, $\beta(x)$ *non-decreasing, if and only if* $\{u_n\}$ *is c.m.*

Property H indicates a relationship between the theory of convergence acceleration and the theory of moments (with a density that depends on the sequence) that is very different from the relationship via Gauss quadrature which is a subject of this paper. In the latter the densities $w^X(\omega), X = P, A, L, M$, do not depend on the series. Hausdorff's original application of completely monotonic sequences has a third, very different, relationship to the summability of sequences, see, e.g., Hardy [8, 1949, Ch. 11].

For applications of higher monotonicity concepts to the construction of rigorous error bounds for numerical methods, see Ström [11, 1970].

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We also refer to the complete bibliography in Part I of this work, in this volume of BIT.