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Numerical inversion of Laplace transforms using integration and convergence acceleration

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Abstract

This report describes a computational scheme for the numerical inversion of Laplace transforms in the case when all singularities occur on the real line. The determination of the value of the inverse function at a given point t proceeds in four major steps:

- Using the Bromwich inversion formula the inverse is represented as an integral over an infinite interval.
- By means of the trapezoidal rule this integral is written as an infinite sum.
- The sum is converted to a power series.
- This power series is evaluated using convergence acceleration.

In order to carry out the last step in an efficient way an aggregation of terms is employed to ensure stability and rapid convergence. The truncation error decreases exponentially with the number of terms used and this fact may be exploited in error estimation and the selection of corresponding parameters in the computer programs. If certain general conditions are satisfied, then only a finite number of parameters is required to specify a function with a preselected accuracy. Thus the values of the inverse transform are calculated on a finite grid, and the transform is determined at all other points with interpolation. It is described how to construct the grid to guarantee that the resulting error does not surpass a bound, defined by the user. An inversion routine based on the ideas put forth in this report has been developed for use with the PROPER code package.

Contents

Summary

The present report consists of three chapters. The first Chapter, Sections 1 through 5, gives a general description of the computational schemes and the principal ideas underlying them. Section 1.1 reminds the reader about some basic mathematical properties of the Laplace transform, which are essential for the efficient use of Laplace transform inversion methods. We introduce Bromwich's formula and mention alternative treatments. Section 1.2 provides basic facts about numerical integration over infinite intervals and the third Section deals with convergence acceleration. It is pointed out that e. g. the ϵ algorithm by Wynn (See e.g. [16]) could be chosen instead of the Chebyshev algorithm. In Section 1.3 we also find the tables which are used for estimating round-off and truncation errors and which govern the setting of certain parameters in the computational schemes. Section 1.4 deals with the tabulation of the inverse Laplace transform. It is intended that these four Sections should provide all necessary information for inverting Laplace transforms, using the codes described in the manual [6]. In Section 1.5 we treat illustrative numerical examples.

Chapter II is devoted to an account for the results from numerical mathematics, upon which the computational schemes are based. In Section 2.1 we define convergence speed and introduce the classes of slowly, geometric and rapidly converging sequences. In Section 2.2 we discuss the summation of rapidly converging sequences in the presence of round-offs, which may mask the true convergence behaviour. The influence of round-offs is further discussed in Section 2.3 where it is proved that term-by-term summation of conditionally convergent series is an unstable process. In Section 2.4 we present a simple and general way of deriving linear convergence acceleration schemes and in Section 2.5 an important special case is treated. In Section 2.6 issues about the stability of these schemes are addressed. In this section we also describe how aggregation improves the stability and convergence of the Chebyshev method. In Section 2.7 we present results about the convergence rates of linear acceleration methods, generalising earlier results in [4]. Sufficient, fairly general conditions guaranteeing that the transformed series has geometric convergence are given.

We have collected some general results from mathematical analysis in Chapter III. In Section 3.1 we give Newton's interpolation formula with remainder and in Section 3.2 Cauchy's integral formula. In Section 3.3 we

discuss the concept of functional recovery and describe how to determine the value of a function at any point of the interval under consideration with a guaranteed accuracy using expressions involving a known number of parameters.

Chapter 1

A computational scheme for Laplace transform inversion

1.1 Some general properties of Laplace transforms

Let f be a real-valued function, which is defined for nonnegative arguments t. Further, f is required to be continuous and of bounded variation on all closed and bounded sub-intervals of $[0, \infty]$. Put

$$F(z) = \int_0^\infty e^{-zt} f(t)\, dt. \tag{1.1.1}$$

As known, F is called the Laplace transform of f. It is analytic on subregions of the complex plane, provided the integral (1.1.1) converges absolutely for some finite z. See Widder, [15]. We note that

$$F(\bar{z}) = \overline{F(z)}, \tag{1.1.2}$$

where, as usual, $\bar{z}$ is the complex conjugate of z. Sometimes we write

$$(\mathcal{L}f)(z) = F(z), \tag{1.1.3}$$

where F is defined by (1.1.1). We note that (1.1.1) defines a *linear mapping*, i.e.

$$\mathcal{L}(f_1 + f_2) = \mathcal{L}f_1 + \mathcal{L}f_2, \quad \mathcal{L}(wf) = w\mathcal{L}f,$$

provided the integrals defining the Laplace transforms of the functions f, f_1 and f_2 do exist.(w is here an arbitrary complex number). Often a differential or integral equation involving a function f may be transformed into a simpler relation involving $\mathcal{L}f$ In some important situations, the integral (1.1.1) may be solved analytically and sometimes one may also find f when $\mathcal{L}f$ is given as an analytic formula. Frequently, however, one must resort to numerical methods. To tabulate F in (1.1.1) given f, is generally a nontrivial task, involving numerical integration over infinite intervals. Here we shall treat the at least equally challenging problem of recovering f, given F. This latter problem has been treated by many authors. See e.g. [2], [8] and [13]. We shall here assume that F is defined by means of a computer program and that the evaluation of F at a given z is expensive. Hence it is desirable to minimise the number of such evaluations. From the outset we shall require that F is analytic everywhere except possibly at points z of the real line satisfying

$$\Re(z) \ < A, \tag{1.1.4}$$

where A is a known real number.

Example 1.1.1

$$f(t) = e^{-t} \ \ F(z) = 1/(z+1) \ \Rightarrow A = \ -1. \tag{1.1.5}$$

Under the general assumptions on F and f described above, **the Bromwich inversion formula** holds:

$$f(t) = \frac{1}{2\pi i}\int_{\Gamma} e^{zt}F(z)\,dz, \tag{1.1.6}$$

where the line Γ is given by

$$\Gamma = \{z \mid z = \gamma + iy, \quad -\infty < y < \infty\}, \tag{1.1.7}$$

and the real constant γ in (1.1.7) must be such that $\gamma > A$. Thus the line Γ is parallel with the imaginary axis. It is essential that F is analytic on Γ and the half-plane to the right of Γ, since otherwise an erroneous value of f will generally result from the numerical schemes to be described. We transform (1.1.6) to an integral involving real arguments as follows. Set

$$\gamma = \gamma_0 + \gamma_1, \tag{1.1.8}$$

where $\gamma_1 > 0$ and γ_0 is the real part of the right-most singular point of F. Then we get

$$f(t) = \frac{e^{t(\gamma_0+\gamma_1)}}{2\pi} \int_{-\infty}^{\infty} e^{iyt} F(\gamma_0 + \gamma_1 + iy)\, dy.$$

Put next $yt = \eta$ and then again $\eta = y$. Then we obtain

$$f(t) = \frac{e^{t\gamma_0}}{2\pi t} e^{t\gamma_1} \int_{-\infty}^{\infty} e^{iy} F(\gamma_0 + \gamma_1 + iy/t)\, dy. \tag{1.1.9}$$

Here γ_0, the position of the right-most singular point of F, is a characteristic of this function but the parameter γ_1 may be chosen. We assume that F may be calculated with the same relative accuracy for all arguments. Our task is to construct a table of f such that $f(t)$ may be determined by interpolation in this table and that $f(t)$ is to be evaluated for a large range of t-values, say for $t = 10^k$, $k = -6, -5, \ldots, 6$. To illustrate the situation we consider

$$F(z) = \frac{1}{1+z}. \tag{1.1.10}$$

As stated in Example 1.1.1, $f(t) = e^{-t}$ and $\gamma_0 = -1$. Hence (1.1.9) becomes

$$f(t) = \frac{e^{-t}}{2\pi} \cdot e^{t\gamma_1} \cdot \int_{-\infty}^{\infty} e^{iy} \frac{1}{\gamma_1 t + iy}\, dy. \tag{1.1.11}$$

In this particular example, (1.1.11), the integral can be calculated exactly with analytic methods but in the general case numerical evaluation must be used. Assume that this is done and that the resulting absolute error in the calculated value is $\epsilon(t)$. Denote the corresponding error in $f(t)$ by $\delta f(t)$. Then we find

$$\delta f(t) = \frac{\epsilon(t) e^{-t}}{2\pi} \cdot e^{t\gamma_1}.$$

Since in this case $f(t) = e^{-t}$, we find the following expression for the relative error

$$\frac{\delta f(t)}{f(t)} = \frac{\epsilon(t)}{2\pi} \cdot e^{t\gamma_1}.$$

The last factor increases unboundedly when $t \to \infty$ for each *fixed* γ_1. Example (1.1.1) also illustrates a general dilemma: small values of γ_1 make the integration difficult, while the right-most singularity of the integrand lies close to the line B and large values of γ_1 cause the factor $e^{\gamma_1 t}$ to grow rapidly with t. Therefore one may let γ_1 depend on t and the choice $\gamma_1 = 1/t$ has been tested with success on many numerical examples. With this choice of γ_1 we have $t\gamma_1 = 1$ and (1.1.9) takes the form

$$f(t) = \frac{e^{t\gamma_0+1}}{2\pi t}\int_{-\infty}^{\infty} e^{iy} F(\gamma_0 + (1+iy)/t)\,dy, \tag{1.1.12}$$

and in the special case of Example 1.1.1

$$f(t) = \frac{e^{-t+1}}{2\pi}\cdot\int_{-\infty}^{\infty} e^{iy}\frac{1}{1+iy}\,dy. \tag{1.1.13}$$

The integral of (1.1.13) is independent of t. We shall demonstrate in Example 1.5.1 how its numerical evaluation may be carried out using general computational schemes. Since the exact value is known, we may study the performance of these schemes on this particular example.

Remark 1.1.1 *The line Γ in (1.1.6) may be replaced by another suitable curve. In [14] a particular choice is discussed in great detail. Other approaches to the problem of inverting Laplace transforms may be found in the survey paper ([2]).*

1.2 Trapezoidal rule over infinite intervals

The integral (1.1.9) cannot, in general, be calculated analytically. Instead, a numerical method is called for, and it is essential that the calculation scheme can be implemented in a computer program, which delivers accurate results for the class of functions to be treated. We note, that the range of integration is unbounded and that the integrand may decay slowly as is illustrated by (1.1.13). Here the integrand is

$$e^{iy}G(y),\ G(y) = \frac{1}{\gamma_1 t + iy}.$$

Assume, for simplicity that $\gamma_1 t = 1$, as recommended in the end of Section 1.1. Thus

$$G(y) = \frac{1}{1+iy}.$$

Thus $G(0) = 1$ and $|G(y)| \leq 10^{-6}$ for all $|y| \geq Y$, if we choose $Y \geq 10^6$. (A lesser value of Y would not do).

Thus the approach to replace the infinite interval in (1.1.9) and (1.1.11) with a bounded range and neglect the contributions from the tails does not appear promising. Instead we shall choose a different route. To facilitate the argument to follow we rewrite the integral of (1.1.9) in the form

$$g(t) = \int_{-\infty}^{\infty} e^{iy} G(y,t)\, dy, \tag{1.2.1}$$

with

$$G(y,t) = F(\gamma_0 + \gamma_1 + iy/t).$$

Thus G is defined by F and depends on γ_0, γ_1 and t and

$$G(-y,t) = \overline{G(y,t)}.$$

We shall also require that the integrand of (1.2.1) and all its derivatives tend to 0 as $|y| \to \infty$.

The integral (1.2.1) is approximated by means of the trapezoidal sum

$$T_h(t) = h \sum_{n=-\infty}^{\infty} e^{inh} G(nh,t), \tag{1.2.2}$$

where h is a positive number to be chosen. Thus the integral (1.2.1) has been approximated by an infinite series (1.2.2). Very many terms would be required to calculate $T_h(t)$ by approximating the series with a partial sum. In many cases, such as (1.1.11) this term by term summation can also be shown to be numerically unstable and hence give unpredictable results. In the Sections to follow we shall describe how to evaluate the series (1.2.2) using convergence acceleration, achieving large gains in speed, accuracy and reliability.

When we replace $g(t)$ with $T_h(t)$, we cause an error, which depends on the step-size h. Put

$$\epsilon(h,t) = g(t) - T_h(t).$$

Using the theory in [12] we may prove:

$$\lim_{h \to 0} \frac{\epsilon(h/2,t)}{\epsilon(h,t)} = 0.$$

This fact justifies the estimate

$$|T_h(t) - g(t)| \approx |T_h(t) - T_{h/2}(t)|. \tag{1.2.3}$$

Thus in order to estimate the error in the approximation

$$T_h(t) \approx g(t),$$

we need to calculate $T_{h/2}$. In the absence of round-offs, $T_{h/2}$ is generally a far better approximation for $g(t)$ than is $T_h(t)$. However, in actual computations, the limited accuracy of computer calculations determines the accuracy obtainable. We propose the following stopping rules:

Choose an $h_0 > 0$ and put

$$h_m = 2^{-m} h_0, \quad m = 0, 1, \cdots, N.$$

A smallest step-size h_N is selected to ensure that the calculations always stop after a finite time. Next calculate

$$\tilde{T}_{h_m}(t), \quad m = 0, 1, \ldots,$$

where $\tilde{T}_{h_m}(t)$ denotes the calculated value of $T_{h_m}(t)$. Accept $\tilde{T}_{h_m}(t)$ as approximation for $g(t)$ for the smallest $m < N$ such that

$$|\tilde{T}_{h_{m+1}}(t) - \tilde{T}_{h_m}(t)| \geq |\tilde{T}_{h_m}(t) - \tilde{T}_{h_{m-1}}(t)|. \tag{1.2.4}$$

If (1.2.4) is not satisfied for any $r < N$, then $\tilde{T}_{h_N}(t)$ is accepted as an approximation for $g(t)$. This strategy has been used with success in numerical work.

Remark 1.2.1 *The integral (1.1.1) may also be evaluated using the trapezoidal rule. It is generally advantageous, first to make the variable transformation*

$$t = e^u.$$

Then (1.1.1) becomes

$$F(z) = \int_{-\infty}^{\infty} e^{u - z \exp u} f(e^u)\, du,$$

and the trapezoidal rule gives the approximation $F_h(z)$ defined by

$$F_h(z) = h \cdot \sum_{n=-\infty}^{\infty} e^{nh - z \exp hn} f(e^{hn}).$$

The discretisation error depends on the step-size h and this error is estimated in the same way as described above for (1.2.1).

1.3 Summation of power series with Chebyshev acceleration

We now discuss how to evaluate the sum (1.2.2) in an efficient way. Setting

$$z = e^{ih}, \tag{1.3.1}$$

and using the fact that

$$G(-nh,t) = \overline{G(nh,t)}, \tag{1.3.2}$$

we immediately find

$$T_h(t) = h[g(0,t) + 2 \cdot \Re(z \cdot \mathcal{G}(z))], \tag{1.3.3}$$

where we have put

$$\mathcal{G}(z) = \sum_{n=0}^{\infty} z^n G((n+1)h,t). \tag{1.3.4}$$

In our notation $\mathcal{G}(z)$ we have suppressed the dependence on t as indicated by (1.3.4). Thus our main task is to evaluate the power series (1.3.4) for different values of t and z. In order to get an accurate approximation of the integral (1.2.1) by the sum (1.2.2) written as (1.3.3) we need to choose the step-size h small. However, the relation (1.3.1) shows, that $h \to 0$ implies $z \to 1$. As discussed in e.g. [4], the problem of calculating the sum of a power series from the numerical values of the first few terms becomes less stable when z approaches 1. Then most convergence acceleration methods give inaccurate results. To counteract this effect an aggregation (or batching) method is used: Let $k \geq 1$ be a fixed integer. Next introduce the k functions $\mathcal{G}_1, \mathcal{G}_2, \ldots, \mathcal{G}_k$ which are defined by

$$\mathcal{G}_r(z) = z^{r-1} \sum_{n=0}^{\infty} z^{nk} G((nk+r)h,t), \quad r = 1, \ldots, k. \tag{1.3.5}$$

Combining (1.3.4) and (1.3.5) we obtain

$$\mathcal{G}(z) = \sum_{r=1}^{k} \mathcal{G}_r(z). \tag{1.3.6}$$

We note that $\mathcal{G}_r$ is a power series with the argument z^k and our aim is to select k such that the series is easier to evaluate than $\mathcal{G}$, which has the argument z. Instead of evaluating 1 series with argument z we evaluate k series with argument z^k. The latter task may be simplified as follows. We rewrite (1.3.4) as

$$\mathcal{G}(z) = \sum_{n=0}^{\infty} \sum_{r=1}^{k} z^{nk+r-1} G((nk+r)h, t),$$

or

$$\mathcal{G}(z) = \sum_{n=0}^{\infty} z^{nk} a_n(z), \tag{1.3.7}$$

where

$$a_n(z) = \sum_{r=1}^{k} z^{r-1} G((nk+r)h, t).$$

In our convergence acceleration scheme we treat (1.3.7) as a power series with argument z^k and coefficients $a_n(z)$, disregarding the fact that these coefficients depend on the argument z. For linear acceleration schemes like those presented in [4] the result of accelerating (1.3.7) is identical to that obtained from accelerating each $\mathcal{G}_r(z)$ individually and adding the results. Also, the nonlinear epsilon algorithm by Wynn, which is described in [16] has been used successfully on series of the type of (1.3.7). We discuss now the proper selection of k in (1.3.7) for the accurate summation of the series (1.3.4). As a consequence of our assumptions on F introduced in the text before (1.1.4) the theory in [4] is applicable for G and we can state:

Theorem 1.3.1 *Let G in (1.3.4) satisfy the assumptions made above. Then the following relations hold:*

$$|R_n(z)| \le E_n(z)\, C, \quad E_n(z) = c(z)|\lambda^n(z)|, \tag{1.3.8}$$

$$|U_n(z)| \le A_n(z)\, D\epsilon, \tag{1.3.9}$$

where

- *$R_n(z)$ is the truncation error, i.e. the difference between the exact sum and the result of performing Chebyshev acceleration, using n terms and assuming that the calculations are carried out exactly.*

- $|\lambda(z)|$ *is called the error factor. It does not depend on* n.

- *The constants* C *and* D *depend on the function* G *but not on* z, n *or* ϵ.

- *The nonnegative function* $c(z)$ *is independent of* n.

- ϵ *is a bound on the absolute error in the terms of (1.3.4).*

- $|U_n(z)|$ *is a bound for the error caused by uncertainties in data, i.e. the values of the terms.*

- $A_n(z)$ *is* z*-dependent factor in* $U_n(z)$.

Remark 1.3.2 *Thus* $|E_n(z)|$ *gives an estimate of the relative error in our estimate of the sum in the absence of round-offs, while* $A_n(z)$ *measures the sensitivity for uncertainty in the input data, that is the terms in (1.3.4). We note that the transformed series converges like a geometric series with quotient* $|\lambda(z)|$.

Summary of strategies for evaluating the integral of (1.1.9) We need to select three parameters namely the step-size h, the number of terms n used for convergence acceleration and k, the number of terms in the aggregation (1.3.6). This can be done using the Tables 1.3.1 and 1.3.2 in this Section. They assume that h is of the form

$$h = \frac{\pi}{2^m}, \quad m = 0, 1, \ldots, 4. \tag{1.3.10}$$

As pointed out in Section 1.2 we introduce a discretisation error when the integral (1.2.1) is approximated by the infinite sum (1.2.2) and this error can only be controlled by decreasing h. We recommend using the halving strategy described in Section 1.2. Thus for each h we need to evaluate the series (1.2.1). If we use Chebyshev acceleration, the transformed series converges like a geometric series. However, we see from Table 1.3.2 that the influence of round-offs not only increases with n, the number of terms transformed, but it increases when we make h smaller. We note also that if we use aggregation according to (1.3.5) through (1.3.7) we replace the original series with argument $z = \exp(ih)$ with another series with argument $z = \exp(ikh)$. Hence we get a more accurate estimation of the sum but instead of n functional values we need to calculate kn such values. We recommend that k is selected such that $z = i$ in the aggregated series.

Example 1.3.3 Assume that $h = \pi/16$. The corresponding values of the $E_n(z)$ and $A_n(z)$ are found in the right-most columns of Tables 1.3.1 and 1.3.2 Thus if we pick $n = 24$ we find $A_n(z) = 0.45E + 12$, which corresponds to a loss of about 12 decimal figures in input data. It does not do much good that $E_n(z) = 0.75E - 06$, promising a good estimate, if the calculations were carried out with infinite precision. Instead we aggregate, taking $k = 8$ and the values in the second columns of the tables apply. If we then choose $n = 10$ we find $E_n(z) = .46E - 06$ and $A_n(z) = .14E + 02$ indicating a loss of a little more than 1 decimal figure in input data. To achieve this we had to calculate $8 \cdot 10$ functional values. It could be argued that the aggregated series (1.3.7) is not the same as the original one but this may be accounted for by multiplying the error bounds by k, in this case 8.

	$m=0$	$m=1$	$m=2$	$m=3$	$m=4$
$n=1$	$.33E+00$	$.45E+00$	$.68E+00$	$.88E+00$	$.96E+00$
$n=2$	$.59E-01$	$.94E-01$	$.19E+00$	$.37E+00$	$.63E+00$
$n=3$	$.10E-01$	$.20E-01$	$.60E-01$	$.15E+00$	$.32E+00$
$n=4$	$.17E-02$	$.44E-02$	$.19E-01$	$.65E-01$	$.17E+00$
$n=5$	$.30E-03$	$.96E-03$	$.58E-02$	$.28E-01$	$.92E-01$
$n=6$	$.51E-04$	$.21E-03$	$.18E-02$	$.12E-01$	$.50E-01$
$n=7$	$.88E-05$	$.45E-04$	$.56E-03$	$.50E-02$	$.27E-01$
$n=8$	$.15E-05$	$.98E-05$	$.17E-03$	$.21E-02$	$.14E-01$
$n=9$	$.26E-06$	$.21E-05$	$.54E-04$	$.89E-03$	$.78E-02$
$n=10$	$.44E-07$	$.46E-06$	$.17E-04$	$.38E-03$	$.42E-02$
$n=11$	$.76E-08$	$.10E-06$	$.52E-05$	$.16E-03$	$.23E-02$
$n=12$	$.13E-08$	$.22E-07$	$.16E-05$	$.68E-04$	$.12E-02$
$n=13$	$.22E-09$	$.47E-08$	$.50E-06$	$.29E-04$	$.66E-03$
$n=14$	$.38E-10$	$.10E-08$	$.16E-06$	$.12E-04$	$.36E-03$
$n=15$	$.66E-11$	$.22E-09$	$.48E-07$	$.52E-05$	$.19E-03$
$n=16$	$.11E-11$	$.48E-10$	$.15E-07$	$.22E-05$	$.10E-03$
$n=17$	$.19E-12$	$.10E-10$	$.46E-08$	$.94E-06$	$.56E-04$
$n=18$	$.33E-13$	$.22E-11$	$.14E-08$	$.40E-06$	$.30E-04$
$n=19$	$.57E-14$	$.49E-12$	$.45E-09$	$.17E-06$	$.16E-04$
$n=20$	$.98E-15$	$.11E-12$	$.14E-09$	$.72E-07$	$.89E-05$
$n=21$	$.17E-15$	$.23E-13$	$.43E-10$	$.31E-07$	$.48E-05$
$n=22$	$.29E-16$	$.50E-14$	$.13E-10$	$.13E-07$	$.26E-05$
$n=23$	$.49E-17$	$.11E-14$	$.42E-11$	$.55E-08$	$.14E-05$
$n=24$	$.85E-18$	$.23E-15$	$.13E-11$	$.23E-08$	$.75E-06$

Table 1.3.1 $E_n(z)$ in (1.3.8) for $h = \pi/2^m \quad z = \exp ih$

	$m=0$	$m=1$	$m=2$	$m=3$	$m=4$
$n=1$	$.67E+00$	$.89E+00$	$.14E+01$	$.18E+01$	$.19E+01$
$n=2$	$.14E+01$	$.18E+01$	$.27E+01$	$.41E+01$	$.60E+01$
$n=3$	$.21E+01$	$.28E+01$	$.49E+01$	$.91E+01$	$.17E+02$
$n=4$	$.28E+01$	$.40E+01$	$.79E+01$	$.20E+02$	$.50E+02$
$n=5$	$.35E+01$	$.52E+01$	$.13E+02$	$.49E+02$	$.16E+03$
$n=6$	$.42E+01$	$.65E+01$	$.21E+02$	$.12E+03$	$.49E+03$
$n=7$	$.49E+01$	$.80E+01$	$.38E+02$	$.29E+03$	$.15E+04$
$n=8$	$.57E+01$	$.97E+01$	$.66E+02$	$.72E+03$	$.48E+04$
$n=9$	$.64E+01$	$.12E+02$	$.12E+03$	$.18E+04$	$.15E+05$
$n=10$	$.71E+01$	$.14E+02$	$.21E+03$	$.44E+04$	$.48E+05$
$n=11$	$.78E+01$	$.16E+02$	$.38E+03$	$.11E+05$	$.15E+06$
$n=12$	$.85E+01$	$.19E+02$	$.68E+03$	$.27E+05$	$.47E+06$
$n=13$	$.92E+01$	$.23E+02$	$.12E+04$	$.66E+05$	$.15E+07$
$n=14$	$.99E+01$	$.27E+02$	$.22E+04$	$.16E+06$	$.47E+07$
$n=15$	$.11E+02$	$.32E+02$	$.40E+04$	$.41E+06$	$.15E+08$
$n=16$	$.11E+02$	$.39E+02$	$.72E+04$	$.10E+07$	$.46E+08$
$n=17$	$.12E+02$	$.48E+02$	$.13E+05$	$.25E+07$	$.15E+09$
$n=18$	$.13E+02$	$.59E+02$	$.24E+05$	$.62E+07$	$.46E+09$
$n=19$	$.13E+02$	$.72E+02$	$.43E+05$	$.15E+08$	$.14E+10$
$n=20$	$.14E+02$	$.89E+02$	$.78E+05$	$.38E+08$	$.46E+10$
$n=21$	$.15E+02$	$.11E+03$	$.14E+06$	$.93E+08$	$.14E+11$
$n=22$	$.16E+02$	$.14E+03$	$.25E+06$	$.23E+09$	$.45E+11$
$n=23$	$.16E+02$	$.17E+03$	$.46E+06$	$.57E+09$	$.14E+12$
$n=24$	$.17E+02$	$.21E+03$	$.83E+06$	$.14E+10$	$.45E+12$

Table 1.3.2 $A_n(z)$ in (1.3.9) for $h = \pi/2^m \quad z = \exp ih$

1.4 Tabulating the inverse Laplace transform

In the preceding Sections we have described how to evaluate the inverse Laplace transform f at a given point t. However, we want to be able to evaluate f for all positive arguments. The idea is to evaluate f at a finite number of grid-points, and to determine f at other arguments by means of interpolation. In [6] linear interpolation is implemented. We must also have information about the asymptotic behaviour of f for large arguments. In this Section we shall assume that

$$\lim_{t\to\infty} f(t) = 0. \tag{1.4.1}$$

If this condition is not satisfied we will require that it is possible to premultiply f with a suitable known function ω such that the product,

$$\omega(t)f(t),$$

satisfies (1.4.1) and replace f by that product in the argument to follow. The construction of an approximation for f is done in the following way

- Select nonnegative numbers a and b and a positive integer N such that $0 \leq a < b$.
- Determine N grid-points t_i, $\quad i = 1, \ldots, N$ according to

$$t_i = a \cdot q^{i-1}, \quad q^{N-1} = b/a.$$

- Calculate $f(t_i)$, for $i = 1, \ldots, N$.
- Define the new function f^* by putting:

$$f^*(t) = f(a), \quad 0 \leq t \leq a,$$

$$f^*(t) = f(b), \quad t \geq b.$$

For each $t \in [a, b]$ we define $f^*(t)$ as the result of linear interpolation between the two grid-points lying closest to t.

Example 1.4.1

$$f(t) = e^{-2t} \quad a = 0, \; b = 8, \quad N = 7.$$

Thus

$$q = \sqrt{2}.$$

We note that f^* is a continuous function. The goodness of fit could be measured in several different ways. We will choose

$$\|f - f^*\| = \sup_{t\geq 0} |f(t) - f^*(t)|. \tag{1.4.2}$$

We note that (1.4.2) gives an upper bound for the pointwise error when f is approximated by f^*. It is possible to improve the accuracy of the approximation by decreasing a and increasing b and/or N. The latter entity could be increased by replacing N by $2 \cdot N - 1$ for a and b fixed. Then the old grid-points are retained and new ones are introduced in between. Using the theory of linear interpolation it is straight-forward to show that the point-wise interpolation error is decreased by a factor of about 4. Further, the largest error generally occurs in the middle between two interpolation points. Since the interpolation error might be quite different in different parts of the interval $[a, b]$ local refinements strategies, based on the observations above can be developed. (See [6]).

1.5 Numerical examples

Here we report the results of some numerical experiments. All calculations discussed here were carried out on a computer working with relative accuracy $2^{-23} \approx 1.2 \cdot 10^{-7}$ (single precision).

Example 1.5.1 *We discuss the evaluation of the integral in (1.1.13), namely*

$$\int_{-\infty}^{\infty} \frac{e^{iy}}{1+iy}\, dy. \tag{1.5.1}$$

Since in this example the integral does not depend on t we write T_h for $T_h(t)$, etc. Thus (1.3.3) becomes

$$T_h = h[1 + 2\Re(z \cdot \mathcal{G}(z)], \tag{1.5.2}$$

where

$$z = e^{ih}, \;\; \mathcal{G}(z) = \sum_{n=0}^{\infty} z^n G((n+1)h), \tag{1.5.3}$$

and

$$G(nh) = \frac{1}{1+inh}.$$

Let m be a positive integer and put

$$h = \frac{\pi}{2^m},\; m = 0, 1, \ldots,$$

in (1.5.2), (1.5.3). Using these values of h and putting $z = e^{ih}$ the sum (1.5.3) was evaluated by means of the Chebyshev acceleration formulæ in [4], and applying the stopping rules described there i.e. without the aggregation (1.3.5). These rules are analogous to those described in Section 3. The exact value of (1.5.1) is $2\pi/e = 2.3114547$. The resulting errors in the calculated values are given in the Table 1.5.1

$h = \pi/2^m$ m	number of func. values	error in calculated value
0	8	$.36E+00$
1	9	$.43E-01$
2	10	$.77E-03$
3	10	$.15E-03$
4	10	$.13E-02$
5	11	$.69E-02$

Table 1.5.1 Results of evaluating (1.5.3) using step-sizes $h = \pi/2^m$ without aggregation.

We next report the results of evaluating (1.5.1) using aggregation according to (1.3.5) such that the argument z^k becomes i in (1.3.7) while the step-lengths in the original series are the same as in Table 1.5.1. Thus no aggregations is possible for $h > \pi/4$ in the original series. Hence the two first lines in Tables 1.5.1 and 1.5.2 are identical.

step-size $h = \pi/2^m$ m	batch-length k	nbr. of terms in batched series	nbr. of terms in original series	error in calculated value
0	1	8	8	$.36E+00$
1	1	9	9	$.43E-01$
2	2	10	20	$.78E-03$
3	4	12	48	$.48E-06$
4	8	11	88	$.00E+00$
5	16	11	176	$.24E-06$
6	32	12	384	$.72E-06$

Table 1.5.2 Results of evaluating (1.5.3) using step-sizes $h = \pi/2^m$ with aggregation.

We observe that the aggregation gives better accuracy since it decreases the impact of the data-error but that more functional values are required. However, G-values are only required in the interval $[0, 6\pi]$ to determine all the terms used in the original series. Therefore one may approximate G by a polynomial in this interval and if less functional values are required to construct a polynomial approximation which reproduces the G-values with full accuracy then computational effort could be saved in this way. This topic is further discussed in Section 3.3.

We next discuss the problem of inverting

$$F(z) = 1 - z\ln(1 + z^{-1}), \tag{1.5.4}$$

which has the inverse

$$f(t) = \frac{1 - e^{-t}(1+t)}{t^2}. \tag{1.5.5}$$

The relation between f and F may be verified as follows: We have

$$\frac{1}{\tau + z} = \int_0^\infty e^{-zt}e^{-\tau t}\,dt. \tag{1.5.6}$$

Multiply each side of (1.5.6) by τ and then integrate with respect to τ over $[0,1]$ and the stated relation follows. If we evaluate F and f for small values of z^{-1} and t respectively, using standard functions a severe loss of accuracy occurs.

t	number of functional values	calculated) $f(t)$	absolute error	relative error
$.1E-03$	40	$.49996656E+00$	$.12E-06$	$.24E-06$
$.1E-02$	44	$.49966669E+00$	$.89E-07$	$.18E-06$
$.1E-01$	40	$.49667913E+00$	$.00E+00$	$.00E+00$
$.1E+00$	44	$.46788400E+00$	$.30E-07$	$.64E-07$
$.1E+01$	44	$.26424101E+00$	$.12E-06$	$.45E-06$
$.1E+02$	44	$.99950079E-02$	$.19E-08$	$.19E-06$
$.1E+03$	48	$.99998186E-04$	$.18E-08$	$.18E-04$
$.1E+04$	48	$.99956571E-06$	$.43E-09$	$.43E-03$
$.1E+05$	48	$.99491766E-08$	$.51E-10$	$.51E-02$

Table 1.5.3 Results of evaluating (1.5.5) using step-size $h = \pi/8$ with aggregation with batch-length 4.

Instead, it is better to expand these function in Taylor series, which results in power series which are rapidly convergent in the sense of Section 2.1. $f(t)$ was determined for $t = 10^j$, $j = -4, -3, \dots, 4$ using the methods described in preceding Sections. Here we take $\gamma_0 = 0$ and $\gamma_1 = 1/t$. The step-size $h = \pi/8$ was taken and aggregation was performed with $k = 4$ and the results in Table 1.5.3 were obtained. We notice that the absolute error never is greater than $1.2 \cdot 10^{-7}$ but that a certain increase in the relative error occurs for t large. This loss of accuracy could be counteracted by working in double precision.

We now discuss how to recover $f(t)$ for positive arguments using linear interpolation from a finite set of grid-points. This recovery cannot be exact, but the accuracy will be greater the denser grid one wants to use. A geometric grid of the type of Table 1.5.3 is advantageous when one wants to reconstruct f over long interval. Then one uses $\log t$ as independent variable and proceeds as described in Section 1.4. Here we shall discuss how to reconstruct $f(t$ over $[0, 100]$ using linear interpolation and accepting an absolute error not greater than 10^{-5}. We split the interval in the parts $[0, 1]$ and $[1, 100]$. For the first interval we use equi-distant grids, for the second geometrical grids. The same step-length and aggregation are used as before.

Equi-distant grid on $[0, 1]$

f was tabulated in the interval $[0, 1]$ with step-length $1/64 = 0.015625$ The corresponding values in the interval $[0.75, 1]$ are shown in Table 1.5.4. Using this table we can estimate the interpolation error in the table with step-length $1/32$ since the largest interpolation error occurs half-way between grid-points. If we interpolate in the table with $h = 1/32$ to determine $f(63/64)$ we obtain this value by averaging the functional values at $t = 1$ and $t = 31/32$. The difference between this average and the tabulated value at $t = 63/64$ gives an estimate of the interpolation error in a table with step-size $1/32$. The interpolation error in the table with spacing $1/64$ is about $1/4$ of this value. By carrying out the corresponding estimates for all arguments of the form

$$\frac{2n-1}{64}, \; n = 1, \dots, 32,$$

we verify that we may determine f at all points t in $[0, 1]$ with an absolute error not greater than $1 \cdot 10^{-5}$ by interpolating in a table with spacing $1/64$, i.e. we recover f with the stated precision in the interval $[0, 1]$ from a grid containing 65 points. Part of the calculated table is shown in Table 1.5.4

t	$f(t)$
t	$f(t)$
.750000	.308193
.765625	.305209
.781250	.302259
.796875	.299342
.812500	.296457
.828125	.293605
.843750	.290784
.859375	.287994
.875000	.285236
.890625	.282508
.906250	.279811
.921875	.277143
.937500	.274505
.953125	.271896
.968750	.269316
.984375	.266764
1.000000	.264241

Table 1.5.4 Equi-distant table with spacing $1/64 = 0.015625$. Interpolation error less than $\approx 1 \cdot 10^{-5}$

Geometrically spaced grid on $[1, 100]$.

f was tabulated at a geometric grid with 129 points, covering the interval $[0, 1]$. Thus the grid-points were given by

$$t_i = 100^{i/128},\ i = 0, 1, \ldots, 128.$$

The linear interpolation error is estimated in the same way as for the equi-distant table and can be shown to be not greater than $\approx 1 \cdot 10^{-5}$. We note that the average distance between grid-points is ≈ 0.78, i.e. the second grid is, on the average 50 times more sparse than the first. Some grid-points could possible be saved by subdividing the interval $[0, 100]$ in more than two sub-intervals and using different discretisation strategies in each of the sub-intervals. Savings could also be achieved by using quadratic or cubic interpolation instead to recover f-values.

t	$f(t)$
1.000000	.264241
1.036633	.258434
1.074608	.252570
1.113974	.246655
1.154782	.240695
1.197085	.234694
1.240938	.228658
1.286397	.222592
1.333521	.216505
74.989418	.000178
77.736504	.000165
80.584221	.000154
83.536255	.000143
86.596436	.000133
89.768715	.000124
93.057205	.000115
96.466164	.000107
100.000000	.000100

Table 1.5.5 Part of geometrically spaced table with 129 points in $[1, 100]$. Interpolation error less than $\approx 1 \cdot 10^{-5}$

Chapter 2

Some theoretical results on convergence acceleration and approximation

2.1 Some measures of convergence speed of series and sequences

Many computational problems can be reformulated as the task of computing limit values. Thus in Section 1.2 we treated the calculation of integrals by means of the trapezoidal rule with step-size h and the integral sought is the limit value which is obtained when $h \to 0$. For each h we needed to evaluate an infinite power series. In this chapter we shall discuss various methods of calculating limit values and we shall present methods of estimating the errors in calculated results. We start by considering the general situation of a sequence

$$s_1, s_2, \ldots, \tag{2.1.1}$$

such that

$$s = \lim_{n \to \infty} s_n, \tag{2.1.2}$$

is defined. Here $s_1, s_2, \ldots, s_n$ may be calculated numerically and the effort necessary depends on n. Put

$$R_n = s - s_n.$$

Thus

$$s = s_n + R_n. \tag{2.1.3}$$

We often make the approximation

$$s \approx s_n. \tag{2.1.4}$$

Then R_n is the associated *truncation error*, which is unknown in general. Hence we need to derive bounds on R_n using any special properties which the sequence $s_1, s_2, \ldots$ might be established to possess. It should be borne in mind that without any bounds on the truncation error, the estimate s_n does not bring any information of the value of s, even if n is large. Associated with the *sequence* (2.1.1) is a *series* with terms $a_0, a_1, \ldots$ where we define $s_0 = 0$ and

$$a_{r-1} = s_r - s_{r-1}, \quad r = 1, 2, \ldots$$

Hence

$$s_n = \sum_{r=0}^{n-1} a_r. \tag{2.1.5}$$

Note that the sum defining s_n has n terms. We write the series corresponding to the sequence (2.1.1), (2.1.2):

$$s = \sum_{r=0}^{\infty} a_r. \tag{2.1.6}$$

Thus

$$R_n = \sum_{r=n}^{\infty} a_r. \tag{2.1.7}$$

If we now put

$$s \approx s_n,$$

then we shall refer to a_n as *the first neglected term.*

Definition 2.1.1 *The sequence (2.1.1) and the equivalent series (2.1.6) are said to be convergent, if*

$$\lim_{n\to\infty} R_n = 0.$$

The convergence is said to be rapid, if

$$\lim_{n\to\infty} \frac{a_{n+1}}{a_n} = 0,$$

and the convergence is termed geometric (or exponential in n) if

$$\lim_{n\to\infty} \frac{a_{n+1}}{a_n} = q, \quad q \neq 0.$$

Otherwise the convergence is said to be slow.

Remark 2.1.2 *We recall the familiar fact that the requirement*

$$\lim_{n\to\infty} a_n = 0,$$

is not sufficient for convergence. This is illustrated by the example

$$a_n = 1/n, \quad n = 1, 2, \ldots,$$

since in this case we may prove

$$\lim_{n\to\infty} \frac{s_n}{\ln n} = 1.$$

This explains why the definition of convergence itself is expressed in terms of the remainder R_n while the three classes of convergent series could be identified by a condition on the terms a_n, $n = 1, 2, \ldots$

Example 2.1.3 *We illustrate the Definition 2.1.1 with the following four series:*

$$a_n = 1/n!, \tag{2.1.8}$$

$$a_n = \frac{1}{(n+1)^2}, \tag{2.1.9}$$

$$a_n = \frac{0.1^n}{\sqrt{n+1}}, \tag{2.1.10}$$

$$a_n = 0.99^{n^2}. \tag{2.1.11}$$

(2.1.8) and (2.1.11) are rapidly convergent, (2.1.10) is geometrically convergent with $q = 0.1$ and (2.1.9) is slowly convergent.

Lemma 2.1.4 *Let the series (2.1.6) be rapidly convergent. Then the following statements follow from Definition 2.1.1:*

$$\lim_{n\to\infty} \frac{a_n}{R_n} = 1, \tag{2.1.12}$$

$$\lim_{n\to\infty} \frac{R_{n+1}}{R_n} = 0, \tag{2.1.13}$$

There is an N such that

$$|a_{n+1}| < |a_n|, \quad n > N. \tag{2.1.14}$$

Remark 2.1.5 *If (2.1.6) is a rapidly convergent series, then we may use the estimate*

$$R_n \approx a_n. \tag{2.1.15}$$

Lemma 2.1.6 *Let (2.1.6) be geometrically convergent with quotient q such that $|q| < 1$. Then there is an N such that:*

$$|a_{n+1}| < |a_n|, \quad n > N, \tag{2.1.16}$$

and there is a positive constant C with

$$|R_n| < Cq^n, \quad n > N, \tag{2.1.17}$$

$$|R_n| < \frac{|a_n|C}{1-q}. \tag{2.1.18}$$

Note that (2.1.17) implies

$$\log|R_n| < \log C + n \log q,$$

where log is the logarithm with basis 10. This means that by geometrical convergence the number of correct digits in our estimate (2.1.4) grows linearly with n, the number of terms used in forming s_n. For efficient calculation of the limit s it is desirable that the series is either rapidly convergent or geometrically convergent with q in (2.1.17) not much greater than about 0.5. Often a series is transformed to improve its convergence. We shall describe several methods for doing so, resulting in large savings in computational efforts as well as more accurate estimates.

2.2 Numerical summation of rapidly convergent series and sequences in the presence of round-offs

In Definition 2.1.1 we introduced the concept of *rapidly* converging series and sequences and we gave same properties which may be used to determine whether an analytically given series or sequence indeed converges rapidly. Let (2.1.1) be a rapidly converging sequence and let

$$\tilde{s}_1, \tilde{s}_2, \ldots, . \qquad (2.2.1)$$

Since we are using a computer working with a finite accuracy, we can generally not expect the calculated sequence (2.2.1) to be rapidly converging in the sense of Definition 2.1.1. Instead we use our knowledge about the exact, but unavailable sequence (2.1.1) to draw conclusions about our calculated values (2.2.1). We illustrate this idea the following simple

Example 2.2.1 *Consider the sequence (2.1.1) with*

$$s_1 = 1, \quad s_{n+1} = (s_n + 7/s_n)/2, \quad n = 1, 2, \ldots \qquad (2.2.2)$$

The corresponding numerical values are listed in Table 2.2.1

i	s_i
1	1.0000000
2	4.0000000
3	2.8750000
4	2.6548913
5	2.6457670
6	2.6457512
7	2.6457512

Table 2.2.1 The sequence defined in (2.2.2).
We next consider the series (2.1.11) which can be shown to be rapidly convergent. We have namely in this case

$$\frac{a_{n+1}}{a_n} = 0.99^{2n+1} \to 0, \text{when } n \to \infty.$$

We give some numerical results in the following table:

n	a_{n-1}	s_n
1	1.0000000	1.0000000
2	.9900000	1.9900000
3	.9605960	2.9505961
4	.9135174	3.8641133
5	.8514579	4.7155714
10	.4430483	7.7695689
20	.0265648	9.2900343
30	.0002134	9.3398037
38	.0000011	9.3400545
39	.0000005	9.3400555
40	.0000002	9.3400555
41	.0000001	9.3400555

Table 2.2.1 The sequence defined in (1.2.11) for selected values of n.

In these two examples the sequence of calculated values converged to a definite value in each case, That does not occur always, since it is possible to construct sequences where the influence of round-offs increases with n and one seeks an estimate such that the combined effect of truncation and round-off errors is minimal. We therefore recommend using a stopping strategy modelled on the one described on p. 6, Section 1.2 for using the trapezoidal rule over the real line. Here the truncation error decreases rapidly when the step-size h is halved successively but the influence of round-offs can be expected to grow moderately when h is decreased. This is probably the most important instance of the summation of rapidly convergent series to be dealt with in this report.

2.3 Stability of term by term summation of series

Convergence acceleration methods are not always used, maybe because the corresponding theory may be considered unusual or complicated. For an account see e.g. ([1]), ([16]). If super-computers are available it would be tempting to estimate the sum by summing the series term by term. We shall discuss three examples which illustrate that the apparently simplest is not always the best. We discuss the following three examples

$$a_r = \frac{(-10)^r}{r!}, \tag{2.3.1}$$

$$a_r = \frac{(-1)^r}{r+1}, \tag{2.3.2}$$

$$a_r = \frac{1}{(r+1)^2}. \tag{2.3.3}$$

All three series are convergent, the first is even rapidly convergent according to Definition 2.1.1. The two first series are alternating. We define the sequences corresponding to these series according to (2.1.5) Since in these examples the true sums are known, we evaluated the differences between the partial sums and the true limiting values in the two latter examples. The results shown in Tables 2.3.1, 2.3.2 and 2.3.3 emerged.

n	a_{n-1}	s_n
1	1.00000	1.00000
2	−10.00000	−9.00000
10	−2755.73210	−1413.14470
11	2755.73210	1342.58740
12	−2505.21110	−1162.62370
20	−82.20636	−27.70642
25	1.61174	.46418
30	−.01131	−.00291
35	.00003	−.00005
36	−.00001	−.00006
37	.00000	−.00006
38	.00000	−.00006

Table 2.3.1 The sequence defined in (2.3.1) for selected values of n.

n	a_n	s_{n+1}	$s - s_{n+1}$
0	1.0000000	1.0000000	.6449341
1	.2500000	1.2500000	.3949341
2	.1111111	1.3611112	.2838229
3	.0625000	1.4236112	.2213229
4	.0400000	1.4636111	.1813229
5	.0277778	1.4913889	.1535451
6	.0204082	1.5117971	.1331370
7	.0156250	1.5274221	.1175120
8	.0123457	1.5397677	.1051663
9	.0100000	1.5497677	.0951663
100	.0000980	1.6350820	.0098521
200	.0000248	1.6399715	.0049626
300	.0000110	1.6416175	.0033165
400	.0000062	1.6424432	.0024909
500	.0000040	1.6429399	.0019941
600	.0000028	1.6432716	.0016625
700	.0000020	1.6435084	.0014256
800	.0000016	1.6436863	.0012478
900	.0000012	1.6438249	.0011091
1000	.0000010	1.6439358	.0009983
1500	.0000004	1.6442682	.0006659
2000	.0000002	1.6444323	.0005018
3000	.0000001	1.6445948	.0003393
4000	.0000001	1.6447140	.0002201
4500	.0000000	1.6447253	.0002087

Table 2.3.2 The sequence defined in (2.3.2) for selected values of n.

n	a_n	s_{n+1}	$s - s_{n+1}$
0	1.0000000	1.0000000	−.3068528
1	−.5000000	.5000000	.1931472
2	.3333333	.8333334	−.1401862
3	−.2500000	.5833334	.1098138
4	.2000000	.7833334	−.0901862
5	−.1666667	.6166667	.0764805
6	.1428571	.7595238	−.0663766
7	−.1250000	.6345238	.0586234
8	.1111111	.7456349	−.0524877
9	−.1000000	.6456349	.0475123
10000	.0001000	.6931917	−.0000445
20000	.0000500	.6931655	−.0000184
30000	.0000333	.6931564	−.0000092
40000	.0000250	.6931525	−.0000053
50000	.0000200	.6931494	−.0000022
60000	.0000167	.6931478	−.0000006
70000	.0000143	.6931464	.0000008
80000	.0000125	.6931457	.0000015
90000	.0000111	.6931448	.0000024
100000	.0000100	.6931441	.0000031
200000	.0000050	.6931411	.0000061
400000	.0000025	.6931394	.0000077
800000	.0000012	.6931385	.0000086
1000000	.0000010	.6931383	.0000089

Table 2.3.3 The sequence defined in (2.3.3) for selected values of n.
The three series (2.3.1),(2.3.2) and (2.3.3) have the sums e^{-10}, $\ln 2$ and $\pi^2/6$ We note that for large n the calculated partial sums s_n give very poor estimates for the true sums. In the case of Table 2.3.1 even the sign is wrong. To approximate the error in the *calculated* sum with the first neglected term would be incorrect in all three cases. For (2.3.3) we have

$$R_n \approx 1/n.$$

Since (2.3.1) for $n > 10$ and (2.3.2) for all n satisfy the conditions of Leibnitz's theorem it is correct to estimate the truncation error with the first neglected term, provided the calculations are carried out exactly on exact data. In these two cases the influence of round-offs and data-errors in single precision (relative accuracy $\approx 1.2 \cdot 10^{-7}$) are significant but for (2.3.3) this source of error was not equally significant. If n is large, the accumulated effect of round- offs during the addition of many terms could be serious. Modern computers often carry out the calculations of sums and scalar products in double precision. However, the error which is caused by the fact that the terms are represented in a finite precision cannot be eliminated and its effect may be significant. To study this phenomenon we need

Definition 2.3.1 *Let the series (2.1.6) be convergent. The convergence is said to be absolute, if*

$$\sum_{r=0}^{\infty} |a_r| \leq M < \infty. \tag{2.3.4}$$

Otherwise the series is said to be conditionally convergent.

Remark 2.3.2 *Geometrically and rapidly converging series are absolutely convergent.*

Theorem 2.3.3 *Term by term summation of a conditionally convergent series is numerically unstable. If the terms are given with a relative error $\leq e$ then the absolute error in the calculated sum of an absolutely convergent series is bounded by*

$$eM/|s|,$$

where s is defined by (2.1.6) and M by (2.3.4).
Proof. *Let a_r be the exact value of a term, $\tilde{a}_r$ its computer representation. Put*

$$\tilde{a}_r = a_r + \epsilon_r,\ r = 0, 1, \ldots,\ \text{with } |\epsilon_r| \leq |e||a_r|,\ \ r = 0, 1, \ldots$$

Setting

$$\tilde{s_n} = \sum_{r=0}^{n-1} \tilde{a}_r,\ \ s_n = \sum_{r=0}^{n-1} a_r,$$

we find

$$|\tilde{s_n} - s_n| \leq e \sum_{r=0}^{n-1} |a_r|.$$

Letting $n \to \infty$ we immediately reach the desired conclusion upon dividing the limiting relation by s in the case of an absolutely convergent series.

Remark 2.3.4 *In the example (2.3.1) we have* $s = e^{-10}$ $M = e^{10}$ *and hence*

$$|\tilde{s} - s| \leq e \cdot \exp(20).$$

For (2.3.2) we find

$$|\tilde{s_n} - s_n| \leq e \sum_{r=o}^{n-1} 1/(k+1) \approx e \ln n,$$

and hence the influence of the error could grow unboundedly when n *is taken large. In (2.3.3) we get* $s = M = \pi^2/6$ *and hence the influence of data-errors is modest. However, the truncation error is significant, close to* $1/n$.

2.4 Linear transformation based on quadrature and interpolation

Consider the general power series

$$\mathcal{F}(z) = \sum_{r=0}^{\infty} c_r z^r, \tag{2.4.1}$$

where the function $\mathcal{F}$ is defined for those z which are such that the series (2.4.1) converges. It is often advantageous to extend the definition of $\mathcal{F}$ also to such areas in the complex plane where the series is divergent. We next introduce:

Definition 2.4.1 *Let* n *be a positive integer,* $\eta_0(z), \ldots, \eta_{n-1}(z)$ n *numbers, which as indicated may depend on* z. *We call*

$$\mathcal{F}_n(z) = \sum_{r=0}^{n-1} \eta_r(z) c_r, \tag{2.4.2}$$

a linear transformation of the power series (2.4.1).

It is desirable that $\mathcal{F}_n(z)$ should give an approximation to $\mathcal{F}(z)$ and often one seeks to construct sequences of transformations $\mathcal{F}_1(z)$, $\mathcal{F}_2(z), \ldots$ such that

$$\lim_{n \to \infty} \mathcal{F}_n(z) = \mathcal{F}(z).$$

Definition 2.4.2 *Associated with the transformation $\mathcal{F}_n(z)$ we introduce its generating polynomial $Q_n(z;\cdot)$ with argument t given by*

$$Q_n(z;t) = \sum_{r=0}^{n-1} \eta_r(z) t^r. \tag{2.4.3}$$

Sometimes it is easiest to define a linear transformation in terms of its generating polynomial.

Example 2.4.3 *Let w be a real or complex number and consider the polynomial*

$$\frac{1}{1-zw} \sum_{r=0}^{n-1} \left(\frac{zt-zw}{1-zw} \right)^r, \tag{2.4.4}$$

obtained by expanding $(1-tz)^{-1}$ in a Taylor series around $t = w$ and retaining the first n terms. For each w (2.4.4) is a generating polynomial of a linear transformation. We mention the special cases:

- $w = 0$*: term by term summation*
- $w = 1$*: generalised Euler transformation*
- $w = 1/2$*: optimal Taylor acceleration (See [4])*

Thus if the generating polynomial of a linear transformation is given, one may determine the transformation itself by expanding the polynomial in power form. Sometimes it is helpful to work with operators to facilitate the calculations. We introduce

Definition 2.4.4 *Let $c_0, c_1, \ldots,$ be a sequence of numbers. We define*

$$c_{r+1} = Ec_r, \quad c_{r+1} - c_r = \Delta c_r, \quad Ic_r = c_r. \tag{2.4.5}$$

E and Δ are called the shift and difference operators, I the identity operator.

Remark 2.4.5 *We may form powers and polynomials of shift and difference operators. They are linear operators and obey familiar laws for multiplication, e.g.:*

$$\Delta^0 = E^0 = I,$$
$$E^{m+n} = E^m \cdot E^n,$$
$$E^m \cdot \Delta = E^{m+1} - E^m.$$

Lemma 2.4.6 *Let now the linear transformation (2.4.2) have the generating polynomial (2.4.3). Then we may write*

$$\mathcal{F}_n(z) = \sum_{r=0}^{n-1} \eta_r(z) E^r c_0 = Q_n(z; E) c_0. \tag{2.4.6}$$

Thus we replace the argument t in the polynomial with the shift operator E. Using the laws mentioned above we may now derive the well-known recursion formulæ associated with the Euler transformation. See e.g. ([4]). We next show how to derive rational expressions approximating the sum (2.4.1) by fitting linear combinations of geometrical series to this power series. Let namely

$$t_1, t_2, \ldots, t_n, \tag{2.4.7}$$

be n fixed numbers. Next determine the unique solution

$$x_1, x_2, \ldots, x_n, \tag{2.4.8}$$

to the linear system

$$\sum_{i=1}^{n} x_i t_i^r = c_r, \quad r = 0, 1, \ldots, n-1. \tag{2.4.9}$$

Next put

$$\hat{c}_r = \sum_{i=1}^{n} x_i t_i^r, \quad r = 0, 1, \ldots,$$

and set

$$\hat{\mathcal{F}}(z) = \sum_{r=0}^{\infty} \hat{c}_r z^r.$$

We note that

$$\hat{c}_r = c_r, \quad r = 0, 1, \ldots, n-1.$$

We next show that $\hat{\mathcal{F}}(z)$ can equivalently be expressed either as a rational expression with z as variable or as a linear transformation of the power series (2.4.1). We find namely

$$\hat{\mathcal{F}}(z) = \sum_{r=0}^{\infty} \hat{c}_r z^r = \sum_{r=0}^{\infty} \sum_{i=1}^{n} x_i t_i^r z^r = \sum_{i=1}^{n} x_i \sum_{r=0}^{\infty} z^r t_i^r = \sum_{i=1}^{n} \frac{x_i}{1 - z t_i}. \tag{2.4.10}$$

Next we demonstrate that $\hat{\mathcal{F}}(z)$ may be expressed as a linear transformation of the form (2.4.2).

Theorem 2.4.7 *Let $t_1, \ldots, t_n$ be as before and determine $\eta_0(z), \ldots, \eta_{n-1}(z)$ as the solution of the linear system*

$$\sum_{r=0}^{n-1} \eta_r(z) t_i^r = \frac{1}{1 - t_i z}, \quad i = 1, 2, \ldots, n. \tag{2.4.11}$$

Thus we get from the above

$$\hat{\mathcal{F}}(z) = \sum_{i=1}^{n} \frac{x_i}{1 - z t_i} = \sum_{i=1}^{n} x_i \sum_{r=0}^{n-1} \eta_r(z) t_i^r = \sum_{r=0}^{n-1} \eta_r(z) c_r. \tag{2.4.12}$$

Remark 2.4.8 *We note that we determined the numbers x_i by solving a linear system of the same type as that encountered when one seeks to determine the weights of a mechanical quadrature rule while $\eta_r(z)$ were obtained after determining an interpolating polynomial. Since these systems are of Vandermonde type they may be treated by using e.g. the codes in ([3]). In order to obtain bounds on $|\hat{\mathcal{F}(z)} - \mathcal{F}((z)|$ we need to introduce assumptions on the coefficients $c_0, c_1, \ldots$. This topic is dealt with in Section 2.7. The derivations in the present and the two next sections are valid for any sequence.*

2.5 Convergence acceleration based on three term recurrence relations

In this Section we shall derive formulæ for the case when the numbers t_i in (2.4.7) are selected as the zeroes of orthogonal polynomials.

Theorem 2.5.1 *Let $t_1, \ldots, t_n$ be the given numbers and put*

$$P_n(t) = \prod_{i=1}^{n} (t - t_i). \tag{2.5.1}$$

Set

$$Q_n(z; t) = \frac{P_n(1/z) - P_n(t)}{(1 - zt) P_n(1/z)}. \tag{2.5.2}$$

Then Q_n is a polynomial of degree $< n$ in t and such that

$$Q_n(z; t_i) = \frac{1}{1 - z t_i}, \quad i = 1, \ldots, n.$$

Proof:
The numerator of the right hand side of (2.5.2) is a polynomial of degree n in t and has a zero at $t = 1/z$. The denominator is a constant multiple of the factor $1/z - t$. Hence $Q_n(z;\cdot)$ is a polynomial of degree $< n$ as claimed. Next $P_n(t_i) = 0$ and therefore

$$Q_n(z;t_i) = \frac{1}{1-zt_i}, \quad i = 1,2,\dots,n,$$

as asserted.

Remark 2.5.2 *Combining (2.4.2), (2.4.12) and (2.5.2) we have*

$$\mathcal{F}_n(z) = \sum_{i=1}^{n} \frac{x_i}{1-zt_i} = Q_n(z;E)c_0. \tag{2.5.3}$$

We now introduce a sequence of polynomials $\mathcal{P}_0, \mathcal{P}_1, \dots$ such that

$$\mathcal{P}_0(t) = 1, \;\; \mathcal{P}_1(t) = t - \alpha_1, \;\; \mathcal{P}_n(t) = (t-\alpha_n)\mathcal{P}_{n-1}(t) - \beta_n \mathcal{P}_{n-2}(t), \;\; n = 2, \dots, \tag{2.5.4}$$

where $\alpha_n, \;\; \beta_n$ are given constants. Next define the polynomial sequence $Q_0(z;\cdot), Q_1(z;\cdot), \dots$ from the relation

$$Q_n(z;t) = \frac{\mathcal{P}_n(1/z) - \mathcal{P}_n(t)}{(1-zt)\mathcal{P}_n(1/z)}. \tag{2.5.5}$$

For the power series (2.4.1) we form the sequence of linear transformations

$$\mathcal{F}_n(z) = Q_n(z;E)c_0, \;\; n = 0, 1, \dots \tag{2.5.6}$$

We next derive a formula for evaluating (2.5.6) for given series (2.4.1) and fixed value of z, by slightly generalising Theorem 1 on p. 62 in ([4]).(Note that we also have opposite sign of z in (2.4.1) and all subsequent definitions)

Theorem 2.5.3 *Use the notations of (2.5.4) and (2.5.5).Put*

$$I_{k,n} = \frac{z^{-k}\mathcal{P}_n(z^{-1}) - E^k \mathcal{P}_n(E)}{I - Ez} c_0. \tag{2.5.7}$$

Then we may use the relations above to establish:

$$\mathcal{F}_n(z,E) = \frac{I_{0,n}}{\mathcal{P}_n(1/z)}, \tag{2.5.8}$$

and $I_{k,n}$ obeys the relations

$$\begin{aligned}
I_{0,0} &= 0, & & (2.5.9)\\
I_{k+1,0} &= (I_{k,0}+c_k)/z, & k=0,1,\ldots & \quad (2.5.10)\\
I_{k,1} &= I_{k+1,0}-\alpha_1 I_{k,0} & k=0,1,\ldots & \quad (2.5.11)\\
I_{k,n} &= I_{k+1,n-1}-\alpha_n I_{k,n-1}-\beta_n I_{k,n-2}, & k=0,1,\ldots,n=2,3, & \quad (2.5.12)
\end{aligned}$$

Remark 2.5.4 *$\mathcal{P}_n(1/z)$ in (2.5.8) is determined using the recurrence (2.5.4) while the numbers $I_{k,n}$ are evaluated in the order $I_{0,0}$, $I_{1,0}$ $I_{0,1}$ $I_{2,0}$, $I_{1,1}$, $I_{0,2}$, etc. Computer programs are listed in ([5]) for the special case when $\mathcal{P}_n$ are the so-called shifted Chebyshev polynomials, i.e. $\alpha_n = 1/2$, $n = 1,2,\ldots,\beta_2 = 1/8$, $\beta_n = 1/16$, $n = 3,4,\ldots$.*

2.6 Stability of linear convergence acceleration schemes

As we showed in Section 2.4 the result of linear transformation of the power series (2.4.1) may be written

$$\mathcal{F}_n(z;E)c_0 = \sum_{r=0}^{n-1} \eta_r(z)c_r. \tag{2.6.1}$$

Let now ϵ_r be the error in the computer representation of c_r where

$$|\epsilon_r| \le \epsilon|c_r|,$$

then we may bound $|U_n(z)|$, the error due to uncertainty in the numerical values of the terms c_r and get the expression

$$|U_n(z)| = |\sum_{r=0}^{n-1} \eta_r(z)\epsilon_r| \le \epsilon \cdot \max_r |c_r| \sum_{r=0}^{n-1} |\eta_r|,$$

proving (1.3.9), if we put

$$D = \max_r |c_r|, \quad A_n(z) = \sum_{r=0}^{n-1} |\eta_r(z)|.$$

Thus in order to determine $A_n(z)$ we only need to determine the sum of the absolute values of the coefficients in the operator polynomial $Q_n(z;\cdot)$. This is done for the case of shifted Chebyshev polynomials and the results are given in Table 1.3.2. We note that the values depend very much on z and that if z is close to 1, then the numerical acceleration becomes unstable. This may be counter-acted by means of aggregation according to (1.3.5) and (1.3.6). Since the absolute values of the terms in the aggregated series is at most k times those of the original series we should multiply the bounds in Table 1.3.2 by k when we use it for estimating the error for an aggregated series.

2.7 On the exponential convergence of some interpolatory acceleration schemes

In this Section we will show that several important linear acceleration schemes give exponential convergence for the transformed series. Our argument depends heavily on the fact that the acceleration schemes are linear, i.e. can be written on the form of (2.4.2). The idea is first to show that the acceleration method under study converges for a certain test-series, whose terms depend on a parameter. Next we show that this test-series generates an entire class of series and this fact is used to extend the convergence proof to this class.

Assume that the terms c_r of the power series (2.4.1) are continuous and differentiable functions of a parameter t. Thus we may write

$$\mathcal{F}(z;t) = \sum_{r=0}^{\infty} c_r(t) z^r, \tag{2.7.1}$$

and

$$\delta_n(z;t) = \mathcal{F}(z;t) - \mathcal{F}_n(z;t) = \mathcal{F}(z;t) - \sum_{r=0}^{n-1} \eta_r(z) c_r(t). \tag{2.7.2}$$

Note that the coefficients $\eta_r(z)$ do not depend on the parameter t. The relations (2.7.1) and (2.7.2) may be differentiated with respect to t to give

$$\frac{\partial \mathcal{F}(z;t)}{\partial t} = \sum_{r=0}^{\infty} c_r'(t) z^r, \tag{2.7.3}$$

and

$$\frac{\partial \delta_n(z;t)}{\partial t} = \frac{\partial \mathcal{F}(z;t)}{\partial t} - \sum_{r=0}^{n-1} \eta_r(z) c_r'(t) z^r. \tag{2.7.4}$$

Likewise, these relations may be integrated. Let ρ be continuous over $[0,1]$ and put

$$d_r = \int_0^1 c_r(t)\rho(t)dt. \tag{2.7.5}$$

Then we get, upon integrating (2.7.1) and (2.7.2) over $[0,1]$

$$\int_0^1 \mathcal{F}(z;t)\rho(t)dt = \sum_{r=0}^{\infty} d_r z^r, \tag{2.7.6}$$

and

$$\int_0^1 \delta_n(z;t)\rho(t)\,dt = \int_0^1 \left(\mathcal{F}(z;t) - \sum_{r=0}^{n-1} \eta_r(z) c_r(t)\right) \rho(t)\,dt. \tag{2.7.7}$$

Example 2.7.1 *Consider the relation*

$$\frac{1}{r+1} = \int_0^1 t^r\,dt. \tag{2.7.8}$$

Thus if we can determine $\delta_n(z;t)$ in (2.7.2) for the geometric test-series with $c_r = t^r$ we can estimate the error which arises when we use the linear transformation in (2.7.1) on the power series

$$\sum_{r=0}^{\infty} \frac{z^r}{r+1}.$$

This result can immediately be generalised. We may differentiate (2.7.8) k times with respect to r to obtain the relation:

$$\frac{k!}{(r+1)^{k+1}} = \int_0^1 t^r (\ln(1/t))^k\,dt, \tag{2.7.9}$$

enabling us to extend the error estimate to a wider class of series. If d_r in (2.7.5) are given analytically as function of r one may sometimes determine ρ. Consider the case when $c_r(t) = t^r$. Then (2.7.5) takes the form

$$d_r = \int_0^1 t^r \rho(t)\,dt. \tag{2.7.10}$$

Next put $t = \exp(-u)$ and we obtain

$$d_r = \int_0^\infty e^{-u(r+1)}\rho(e^{-u})\,du. \tag{2.7.11}$$

Now ρ may, in some favourable cases, be determined from a table of inverse Laplace transforms. This approach could be used to find ρ e.g. for $d_r = 1/(1+r^2)$ and the method may be extended to the case when d_r is a rational and bounded function of r.

Remark 2.7.2 *(2.7.5) may be replaced by the Riemann-Stieltjes integral*

$$d_r = \int_0^1 c_r(t)d\sigma(t), \tag{2.7.12}$$

where the integrator σ is of bounded variation on $[0,1]$. The practical use of this condition in the case $c_r(t) = t^r$ is dealt with in ([4]). General criteria for verifying (2.7.12) in this case can be found in ([15]).

Definition 2.7.3 *Power series of the type (2.4.1) such that the coefficients d_r admit a representation (2.7.5) or more generally (2.7.12) wth $c_r(t) = t^r$ are called moment series.*

We shall now study the convergence properties of linear acceleration formulæ on the power series (2.4.1) when the terms d_r admit the representation

$$d_r = r^\ell \int_0^1 t^r w(t)dt, \quad \ell \geq 0, \text{integer}, \quad r = 0, 1, \ldots. \tag{2.7.13}$$

We therefore introduce test-series with

$$c_r = r^\ell t^r, \ t \text{ fix}, \ \ell \geq 0 \text{ integer}. \tag{2.7.14}$$

Lemma 2.7.4 *Put*

$$\delta_n(z;t) = \frac{1}{1-tz} - \sum_{r=0}^{n-1} \eta_r(z)t^r, \tag{2.7.15}$$

$$\delta_{\ell,n}(z;t) = \sum_{r=0}^{\infty} r^\ell t^r z^r - \sum_{r=0}^{n-1} \eta_r(z) r^\ell t^r. \tag{2.7.16}$$

Then $\delta_{\ell,n}(z;t)$ is obtained from the recurrence relation:

$$\delta_{n,0}(z;t) = \delta_n(z;t), \ d_{n,k+1}(z;t) = t\delta'_{n,k}(z;t), k = 0, 1, \ldots, \ell - 1.$$

Proof
Differentiate (2.7.15) after t and then multiply the relation with t.

Lemma 2.7.5 *Use the notations of Theorem 2.5.1. Using (2.5.1) we verify straight-forwardly:*

$$\delta_n(z;t) = \frac{1}{1-tz} - Q_n(z;t) = \frac{P_n(t)}{(1-tz)P_n(1/z)}. \tag{2.7.17}$$

We also need the following result, which is easily shown by means of Cauchy's integral formula:

Lemma 2.7.6 *Let Ω be a closed and bounded subset of the complex plane such that its boundary is a simple closed contour. Let Γ be a closed simple contour in the interior of Ω and such that the points of Γ are at a positive distance from the boundary of Ω. Denote by Ω^* the subset of Ω which is on or at the inside of Γ. Let further ϕ be analytic on a set, which contains Ω and be such that there is a constant M with the property*

$$|\phi(z)| \leq M, z \in \Omega.$$

Define the sequence ψ_ℓ, $\ell = 0, 1, \ldots,$ according to

$$\psi_0(z) = \phi(z),\ \psi_\ell(z) = z\psi'_{\ell-1}(z), \ell = 1, 2, \ldots, .$$

Then we may prove

$$|\psi_\ell(z)| \leq B_\ell M, \quad z \in \Omega^*,$$

where the constant B_ℓ is independent of ϕ.

We first treat the test-series (2.7.14) for $\ell = 0$. Then we use Lemma 2.7.6 to extend the validity of the error bounds to general ℓ. Finally we apply (2.7.10) to extend the results to a general class of series. We will treat the linear acceleration formulæ defined by (2.4.4)(Taylor expansion) and by the three-terms recurrence relation formula for shifted Chebyshev polynomials (Remark 2.5.4).

Theorem 2.7.7 *Put*

$$\kappa = \max_{0 \leq t \leq 1} \frac{|z(t-w|}{|1-zw|}.$$

If $\kappa < 1$ then (2.4.4) converges exponentially for the test-series (2.7.14) and also for the class of series whose terms satisfy (2.7.5).

Proof.
Setting $t_i = w$, $i = 1, \ldots, n$ in the definition of P_n in (2.5.1) we find from (2.7.17)

$$\delta_n(t; z) = \frac{1}{1 - zt} \left(\frac{z(t-w)}{1 - zw} \right)^n .$$

Thus

$$|\delta_n(t; z)| \leq \frac{\kappa^n}{|1 - zt|}.$$

Since $\kappa < 1$ we may construct an ellipse Γ with foci at 0 and 1 such that

$$\max \frac{|z(t-w)|}{|1 - zw|} \leq \nu, \ \nu = (1 + \kappa)/2 < 1,$$

for all z on Γ or in its interior. Thus we put

$$M = A\nu^n,$$

in Lemma (2.7.6) and conclude that

$$|\delta_n(z; t)| < A\nu^n \ \ \delta_{n,\ell}(z, t) < B_\ell A \nu^n, \ \ 0 \leq t \leq 1,$$

where A, B_ℓ are constants. Thus we have verified exponential convergence for the test-series.

We next verify the exponential convergence for the case of Chebyshev acceleration.

Theorem 2.7.8 *Let $t_i, i = 1, 2, \ldots, n$ in (2.5.1) are the zeroes of the shifted Chebyshev polynomials T_n^*. Then the linear transformation formulæ (2.4.2) converges exponentially for the test-series (2.7.14).*
Proof
We find

$$\delta_n(z, t) = \frac{T_n^*(t)}{(1 - tz) T_n^*(1/z)},$$

where for complex z

$$T_0^*(z) = 1, \ T_1^*(z) = 2z - 1, \ T_n^*(z) = (4z - 2)T_{n-1}^*(z) - T_{n-2}^*(z), \ n = 2, 2, \ldots. \tag{2.7.18}$$

We note that $|T_n^*(t)| \leq 1$ *if* $t \in [0,1]$. *Further (2.7.18) is a difference equation with constant coefficients we find the solution*

$$T_n^*(z) = \frac{1}{2}(\lambda_1^n + \lambda_2^n), \tag{2.7.19}$$

$$\lambda_1 = 2z - 1 + 2\sqrt{z^2 - z}, \quad \lambda_2 = 2z - 1 - 2\sqrt{z^2 - z}. \tag{2.7.20}$$

Thus if $1/z$ *does not belong to* $[0,1]$ *we may conclude the exponential convergence for the test-series (2.7.14) in the case* $\ell = 0$ *from (2.7.19),(2.7.20) To extend this result to the case* $\ell > 0$ *we consider an ellipse with foci in* 0 *and* 1 *but such that* $1/z$ *is outside of the ellipse. Put*

$$\zeta(\theta) = 1/2 + (\mu + \mu^{-1})/4 \quad \mu = Re^{i\theta}, \quad R > 1. \tag{2.7.21}$$

When θ *varies* ζ *describes an ellipse with center at* $z = 1/2$ *and semiaxes* $(R + R^{-1})/4$ *and* $(R - R^{-1})/4$. *Using the difference equation (2.7.18) we find*

$$T_n^*(\zeta) = (\mu^n + \mu^{-n})/2,$$

and hence we may use Lemma 2.7.6 to establish that the Chebyshev acceleration gives exponential convergence for moment series.

Chapter 3

Some general results from the theory of interpolation

3.1 Newton's interpolation formula

One of the main ideas in classical numerical analysis is to approximate functions with polynomials and carry out operations like interpolation, differentiation and integration on these latters. Much effort has been devoted to construction of suitable formulæ for doing this as well as estimating the errors, hereby arising. In this section we have collected some central results and definitions from this area.

Definition 3.1.1 *Let the function ϕ be defined on a set Ω on the real line or in the complex plane. Let $\Omega_N \subset \Omega$ be a fixed subset containing N points. We define the divided differences of ϕ with respect to Ω_N as follows*

one argument: $\phi(z_i)$, $z_i \in S_N$,

two arguments:

$$\phi(z_i, z_j) = \frac{\phi(z_j) - \phi(z_i)}{z_j - z_i}, \quad i \neq j, \tag{3.1.1}$$

k **arguments** *By induction:*

$$\phi(z_{i_1}, \dots, z_{i_k}) = \frac{\phi(z_{i_2}, \dots, z_{i_k}) - \phi(z_{i_1}, \dots, z_{i_{k-1}})}{z_{i_k} - z_{i_1}}, \; k = 2, \dots, \; z_{i_j} \in \Omega_N. \tag{3.1.2}$$

Remark 3.1.2 *Using induction one may verify that the value of a divided difference with k arguments is independent of the order of these arguments. The definition above requires that the arguments are distinct. However, if ϕ has sufficiently many derivatives it is possible to extend the definition to confluent arguments by means of a suitable limiting process, e.g.*

$$\phi(z,z) = \phi'(z).$$

Newton's interpolation formula:

Theorem 3.1.3 *Let ϕ and Ω be as in Definition 3.1.1 and put*

$$\Omega_N = \{z_1, z_2, \ldots, z_N\}.$$

Then for each n such that $1 \le n \le N$ we have:

$$\phi(z) = Q_n(z) + R_n(z), \quad i \in S,$$

where Q_n is the polynomial of degree less than n which satisfies

$$Q_n(z_i) = \phi(z_i), \quad i = 1, 2, \ldots, n,$$

and the remainder R_n has the form

$$R_n(z) = \phi(z, z_1, z_2, \ldots, z_n) \prod_{i=1}^{n} (z - z_i). \tag{3.1.3}$$

Proof:
R_n and Q_n are constructed, using the definition of divided differences. We have namely

$$\phi(z) = \phi(z_1) + (z - z_1)\phi(z, z_1).$$

Thus for $n = 1$ we have $Q_1(z) = \phi(z_1)$ and $R_1(z) = \phi(z, z_1)(z - z_1)$ as claimed. To treat the case $n = 2$ we use:

$$\phi(z, z_1) = \phi(z_1, z_2) + (z - z_2)\phi(z, z_1, z_2).$$

Combining this with the preceding relation we obtain

$$\phi(z) = \phi(z_1) + (z - z_1)\phi(z_1, z_2) + (z - z_1)(z - z_2)\phi(z, z_1, z_2).$$

Hence for $n = 2$ we find

$$Q_2(z) = \phi(z_1) + (z - z_1)\phi(z_1, z_2), \quad R_2(z) = \phi(z, z_1, z_2)(z - z_1)(z - z_2).$$

The constructive part is now completed using an induction argument. The uniqueness of the interpolating polynomial is verified by using contradiction: Let Q^* and Q be polynomials of degree less than n and such that

$$Q^*(z_i) = Q(z_i) = \phi(z_i), i = 1, 2, \ldots, n,$$

i.e. Q^* and Q both solve the interpolation problem. Put

$$V(z) = P = Q^*(z) - Q(z).$$

Then V is a polynomial of degree less than n satisfying

$$V(z_i) = 0, \ i = 1, 2, \ldots, n.$$

This is only possible if V is identically zero, establishing the uniqueness of the solution of the interpolation problem.

We next discuss:

Example 3.1.4 *Put*

$$\phi(z) = \frac{1}{1 - zw}.$$

Then we have

$$R_n(z) = \frac{1}{1 - zw} \frac{\prod_{i=1}^{n} (z - z_i)}{\prod_{i=1}^{n} (1/w - z_i)}.$$

If Ω in Theorem 3.1.3 is a closed and bounded real interval $[a, b]$ and ϕ has n continuous derivatives on Ω then we may prove

$$R_n(z) = \frac{\phi^{(n)}(\xi)}{n!} \prod_{i=1}^{n} (z - z_i), \quad \xi \in [a, b]. \tag{3.1.4}$$

We note that ξ is unknown, and in most applications it is not easy to estimate the magnitude of high-order derivatives. However, the function in Example (3.1.4) occurred in Chapter 2 and we note that an explicit expression for $R_n(z)$ is available in this important case. Also, in the next Section we will show that the task of estimating the high-order derivative may be avoided if we know the value of the function itself on a suitable curve in the complex plane. We also note that $R_n(z)$ in (3.1.4) contains a factor which depends only on the nodes z_i. In fact, it is possible to show:

Theorem 3.1.5 *Let Ω in Theorem 3.1.3 be the closed and bounded interval $[a,b]$ and let ϕ have n continuous derivatives there. Then*

$$|R_n(t)| \leq 2\left(\frac{(b-a)}{4}\right)^n \max_{a\leq t\leq b} \frac{|\phi^{(n)}(t)|}{n!}, \tag{3.1.5}$$

if

$$t_i = \frac{a+b}{2} + \frac{b-a}{2}\theta_i \;\; \theta_i = \pi\frac{n-i+1/2}{n}, \quad i = 1,2,\ldots,n.$$

3.2 Cauchy's integral formula with applications

Definition 3.2.1 *The subset Γ of the complex plane is called a smooth arc if*

$$\Gamma = \{z(t) = x(t) + iy(t) |\; t \in [a,b]\},$$

where x and y are continuously differentiable functions of t on $[a,b]$ and such that

$$|x'(t)| + |y'(t)| > 0 \;\forall t \in [a,b].$$

The arc is called a closed contour if also $z(a) = z(b)$ and otherwise $z(t_1) = z(t_2)$ implies $t_1 = t_2$.

Example 3.2.2

$$z(\theta) = e^{i\theta},\; 0 \leq \theta \leq 2\pi,$$

is the unit circle, and a closed contour

Example 3.2.3 *The closed contour given by*

$$z(\theta) = 1/2\left(Re^{i\theta} + R^{-1}e^{-i\theta}\right) \;\; 0 \leq \theta \leq 2\pi, \;\; R > 1, \tag{3.2.1}$$

is an ellipse with center at the origin, foci at $+1$ and -1 and semi-axes $1/2(R+1/R)$ and $1/2(R-1/R)$.

We now state

Cauchy's integral formula

Theorem 3.2.4 *Let ϕ be analytic on a domain Ω in the complex plane, Γ be a closed contour in S. Then for any z interior to Γ we have*

$$\phi(z) = \frac{1}{2\pi i} \oint_\Gamma \frac{\phi(\zeta)}{\zeta - z} d\zeta. \tag{3.2.2}$$

Remark 3.2.5 *We note that the values of ϕ in the interior of Γ are completely determined from the values on the curve Γ. Hence (3.2.2) could be used for calculating these values. If a smooth parametrisation of the curve is given, then the trapezoidal rule will give accurate estimates of $\phi(z)$, provided z is on some distance from the curve.*

Under the assumptions of Theorem 3.2.4 we may also prove

$$\phi^{(k)}(z) = \frac{k!}{2\pi i} \oint_\Gamma \frac{\phi(\zeta)}{(\zeta - z)^{k+1}} d\zeta. \tag{3.2.3}$$

Hence if we have a bound of the type

$$|\phi(z)| \le M, \ z \in \Gamma.$$

we may determine a bound on the values of all derivatives of ϕ at the interior of Γ. However, these bounds get large, if z is close to the curve Γ. These bounds may be used for estimating the magnitude of the remainder term in Newton's interpolation formula. Combining the definition of divided differences with (3.2.3) we immediately obtain

$$\phi(z, z_1, \ldots, z_n) = \frac{1}{2\pi i} \oint_\Gamma \frac{\phi(\zeta)}{(\zeta - z) \prod_{i=1}^{n} (\zeta - z_i)} d\zeta. \tag{3.2.4}$$

Entering this expression into (3.1.3) we get the following expression for the remainder term R_n of Newton's interpolation formula

$$R_n(z) = \frac{1}{2\pi i} \oint_\Gamma \frac{\phi(\zeta)}{(\zeta - z)} \frac{P_n(z)}{P_n(\zeta)} d\zeta, \tag{3.2.5}$$

where ϕ is interpolated at $z_1, \ldots, z_n$ and

$$P_n(z) = \prod_{i=1}^{n} (z - z_i).$$

We will now show that the interpolation error decreases exponentially in the number of nodes if we use the zeroes of Chebyshev polynomials and certain general conditions are satisfied.

Definition 3.2.6 *The Chebyshev polynomials $T_0, T_1, \ldots,$ satisfy the recurrence relation*

$$T_0(t) = 1,\ T_1(t) = t,\ T_n(t) = 2t \cdot T_{n-1}(t) - T_{n-2}(t),\ n = 2, 3, \ldots \tag{3.2.6}$$

This relation may be considered as a difference equation with constant coefficients. It may be solved for $T_n(t)$ and we may establish that T_n has zeroes at

$$t_i = \cos(\theta_i)\ \ \theta_i = \pi \frac{n - i + 1/2}{n},\ i = 1, 2, \ldots, n. \tag{3.2.7}$$

Straight-forwardly we also verify

$$T_n(1/2(z + 1/z)) = 1/2(z^n + z^{-n}). \tag{3.2.8}$$

We next state:

Theorem 3.2.7 *Let ϕ be analytic on and in the interior of the ellipse (3.2.1) and assume that $|\phi(z)| \leq M$ on this set. Let Q_n be the polynomial of degree less than n which interpolates ϕ at the points t_i defined in (3.2.7). Let*

$$z = 1/2(\zeta + 1/\zeta),\ \ \zeta = R_0 e^{i\theta}, \theta \in [0, 2\pi],\ R_0 < R.$$

Then there is a constant, C independent of R_0, R, n such that

$$|\phi(z) - Q_n(z)| \leq C(R_0/R)^n.$$

Proof: Combine (3.2.5) and (3.2.8)

Remark 3.2.8 *The last theorem may be generalised. Let namely ϕ be analytic in a set, which contains the real interval $[a, b]$ in its interior. Make a change of variable and define ψ according to*

$$\psi(t) = \phi\left(\frac{a + b}{2} + \frac{b - a}{2} t\right).$$

If we now interpolate ψ at the points (3.2.7) the preceding theorem guarantees that the interpolation error decreases exponentially in n. This fact was illustrated by the Chebyshev convergence acceleration schemes discussed in Section 2.7, where $\phi(t) = 1/(1 - tz)$ was interpolated in the interval $[0, 1]$

3.3 Recovery of functional values

We consider in this final section the general problem of evaluating a function with an error which does not surpass a given tolerance. In many situations one can show that a fixed function can be reproduced with a prescribed tolerance using a finite number of parameters. However, the number of parameters depend both on the tolerance accepted and the function to be reproduced as well as the method chosen for the recovery. We illustrate this with

Example 3.3.1 *Let ϕ be twice differentiable on $[0,1]$ and such that $|\phi''(t)| \leq c$ on $[0,1]$. We want to recover ϕ with piece-wise linear interpolation using N functional values. Then the step-size is $h = 1/(N-1)$ and the interpolation error is bounded by*

$$ch^2/8 = \frac{c}{8(N-1)^2}.$$

In the case $\phi(t) = e^{-t}$ we have $c = 1$ and if we take $N = 1200$ the function obtained by piecewise linear interpolation cannot be distinguished from $\phi(t) = e^{-t}$ in single precision. Hence it may replace the given function in all numerical work in single precision which does not depend on functional values outside of $[0,1]$.

We next discuss an example where the given function is not defined by an expression composed of so-called standard functions

Example 3.3.2 *Consider the function*

$$\phi(z) = \sum_{n=0}^{\infty} \frac{z^n}{(n!)^2}, \; |z| \leq 1.$$

For each fixed z the power series is rapidly convergent in the sense of Section 2.1 and if we approximate ϕ with Q_n where

$$Q_n(z) = \sum_{r=0}^{n-1} \frac{z^r}{(r!)^2},$$

then we may set

$$|\phi(z) - Q_n(z)| \approx \frac{|z^n|}{(n!)^2}.$$

Therefore, if we consider such z with $|z| \leq 1$ ϕ and Q_n become indistinguishable in single or in double precision already for n moderate. Hence, for computational purposes the transcendental function can be replaced by a polynomial of moderate degree on the set $|z| \leq 1$.

In section 3.2 we described how functions on bounded intervals could be replaced by polynomials in such a manner that the approximation error decreases exponentially in the degree of the approximating polynomial, i.e. in the number of parameters used. Finally, we will show how functional recovery may be used to save computational work in the inversion of Laplace transforms: Our task may be formulated as the problem of numerically evaluating the integral (1.1.9) for real, positive values of t. To do this we need values of the function F and as follows from the argument in Section 1.2 we need only F-values for $y > 0$. Further we need a table of equi-distant values with spacing h. If we had not used convergence acceleration we would need to tabulate F over vast y-intervals, but the acceleration methods decreases this need significantly. Let the number of functional values used be N (The number of terms in the aggregated series is generally considerably less, but we need functional values to form the original series). Thus we need F-values in an y-interval of length Nh/t. It is important to realise that F-values outside of this interval do not influence the computed value of the integral. Referring back to Table 1.3.1 we find that if we take $h = \pi$, $n = 12$ we get $E_n(z) = 0.13 \cdot 10^{-8}$ while $n = 14$, $h = \pi/2$ gives $E_n(z) = 0.10 \cdot 10^{-8}$, $n = 18$, $H = \pi/4$ gives $E_n(z) = 0.14 \cdot 10^{-8}$. Finally $n = 24$, $h = \pi/8$ implies $E_n(z) = 0.23 \cdot 10^{-8}$. Thus we need F-values in an interval of length $12\pi/t$ to secure that $E_n(z) < 10^{-8}$. Nevertheless, we need many functional values if we need to select h small to get a small discretization error when we approximate the infinite integral with a trapezoidal sum. Then one can use interpolation to construct a simpler function, e.g. a piecewise polynomial which approximates F in this y-interval within the working accuracy of the computer. This is advantageous, if the evaluation of F is expensive and the construction of the approximating function requires fewer functional evaluation than does the calculation of terms used in the convergence acceleration scheme. The fact that the result of the computations is independent of the F-values outside the interval mentioned here, means that it is essential that one has verified mathematically that it is indeed permissible to neglect these outside values, i.e. use convergence acceleration.

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Lists of technical terms and mathematical symbols

The following lists contain some key concepts and terms used in this report, as well as mathematical symbols used. For each entry is given a reference to the page, sometimes formula number, where it occurs for the first time. It is generally defined there. In some cases later occurrences are also given

Subject index

Lower case English letters

a Left end-point of real interval 13

a_r Term in series 20, 21, 22

$a_n(z)$ z-dependent coefficient in the aggregated series (1.3.7) 8

b Right endpoint of real interval 13

$c(z)$ Nonnegative function appearing in (1.3.8) 8

c_r Coefficients in the general power series (2.4.1) 30

$\hat{c}_r$ Coefficients in power series, reconstructed by quadrature 32

$c_r(t)$ Coefficients of the power series (2.7.1), depending on the real variable t 36, 37, 38

d_r Coefficients in integrated power series 37

e Bound for relative error in calculated value of term a_r in Theorem 2.3.3 29

f Real valued function, defined for positive arguments t 1

f^* Approximation to inverse Laplace transform f constructed from data on a finite grid 13

f_1, f_2 Real-valued functions 2

$g(t)$ Integral defined by (1.2.1) 5

h Step-size for trapezoidal approximation (1.2.2) 5, 7, 8, 9, 14, 15

$h_0, h_1, \ldots, h_N$ Sequence of step-sizes for trapezoidal rule with

$$h_r = 2^{-m} h_0,$$

where h_0 is a given initial step-size 6

ℓ Integer 38, 39, 40, 41

m Integer. After m halvings the step-size in the trapezoidal sum is $2^{-m}h_0$ 14

q Quotient defining geometric sequence or terms in geometric series 13, 22

s Limit of sequence or sum of the corresponding series (2.1.2) (2.1.6) 20, 21

s_n element in sequence (2.1.1) 20

s_n partial sum in series (2.1.5) 21

$\tilde{s}_n$ Calculated value of s_n (2.2.1) 24

u Real variable 6

t Real-valued variable

t_i points on the real line 13, 32, 33

w Complex constant (2.4.4) 1, 31, 44

x_i Weight in mechanical quadrature rule

y Real-valued variable

z Complex-valued variable

z_i points in the complex plane 42, 42

Upper case English letters

A Real constant 40

$A_n(z)$ z-dependent factor in $U_n(z)$, bound for influence of uncertainties in the coefficients of the power series (1.3.4) 8, 10, 12

B_ℓ Real constants 39, 40

C Nonnegative constant in (1.3.8) and in (2.1.17) 8, 23

D Nonnegative constant in (1.3.8) 8

E Power of 10. Example: $0.75E - 06 = 0.75 \cdot 10^{-6}$ 10, 11, 12

E Shift operator in (2.4.5) 31

$E_n(z)$ z-dependent factor of truncation error $R_n(z)$ in (1.3.8) 8, 10, 11, 49

F Complex-valued function, the Laplace transform of f, i.e. $F = \mathcal{L}f$ 1

$F_h(z)$ Trapezoidal approximation for $F(z)$ 6

G Complex-valued function, defined in terms of F by

$$G(y,t) = F(\gamma_0 + \gamma_1 + iy/t)$$

4, 5

I Identity operator in (2.4.5) 31

$I_{k,n}$ Number, defined in Theorem 2.5.3 34, 35

P_n Polynomial of degree exactly n, the n zeroes of which are known 33, 46

Q, $Q*$ Polynomials of degrees $< n$ 44

Q_n Polynomial of degree less then n, defining approximation (2.4.3), (2.5.2) 31, 33

R Positive constant 41, 45

R_0 Positive constant 47

R_n Truncation error or remainder term 20

$T_h(t)$ Trapezoidal sum with step-size h (1.2.2) 5

$\tilde{T}_{h_m}(t)$ Calculated value of the trapezoidal sum $T(h_m(t)$ 6

T_n Chebyshev polynomials, defined by the recurrence (3.2.6) 47

T_n^* Shifted Chebyshev polynomials defined by recurrence (2.7.18) 40, 41

$U_n(z)$ Bound for error caused by uncertainties in the coefficients of (1.3.4) 8, 9

V Polynomial of degree $< n$ 44

Y Real number 5

Upper case calligraphic letters

$\mathcal{F}$ General power series defined by (2.4.1) 30, 32, 33, 36, 37

$\mathcal{F}_n(z)$ Linear transformation defined by (2.4.2) 30, 32, 32, 34, 35, 36

$\hat{\mathcal{F}}(z)$ Sum of power series with reconstructed coefficients $\hat{c}_r$ 32, 33

$\mathcal{G}(z)$ Power series defined by (1.3.4) 7, 8, 14

$\mathcal{G}_r(z)$ Power series defined by (1.3.5) 7, 8

$\mathcal{L}$ Operator for Laplace transformation (1.1.3) 1, 2

$\mathcal{P}_n$ Member of sequence of polynomials defined by (2.5.4) 34, 35

Lower case Greek letters

α_n Coefficients in recurrence (2.5.4) 34, 35

β_n Coefficients in recurrence (2.5.4) 34, 35

γ Real constant 2

γ_0, γ_1 Real constants 2, 3, 4, 5, 17

δ $\delta f(t)$ Bound for absolute error in the value of $f(t)$ 3
item[$\delta_n(z;t)$] Truncation error for power series (2.7.1) 36, 37, 38, 39, 40

ϵ Bound for absolute error in coefficients of power series 8, 9, 35

$\epsilon(t)$ Bound for absolute error of calculated integral depending on real variable t 3

$\epsilon(h,t)$ Discretisation error caused by trapezoidal approximation (1.2.2) 5

ϵ_r Absolute error in calculated value of term a_r in Theorem 2.3.3 29, 35

ζ Complex variable 41, 46, 47

η Real variable 3

$\eta_r(z)$ Coefficients in linear transformation formula (2.4.2) They depend on the complex variable z 30, 31, 32, 33, 35, 36, 37, 38

θ Real variable in the interval $[0, 2\pi]$ 41, 45

κ Bound on convergence rate in Theorem 2.7.7 39

$\lambda(z)$ Error factor in (1.3.8). The transformed series converges like a geometric series with quotient $\lambda(z)$ 8, 9

λ_1, λ_2 Characteristic roots of the difference equation (2.7.19) 40

μ Complex variable, defined in (2.7.21) 41

ν Bound on convergence factor in Theorem 2.7.7 40

ξ Real variable 44

ρ Continuous weighting function in (2.7.5) 37, 38

σ Integrator in the Riemann-Stieltjes integral (2.7.12) 38

τ Real variable 16

ϕ Function which is defined on sub-sets of the complex plane 39, 42, 43, 44, 45, 46, 47, 48, 49

ψ_ℓ Functions which are defined on sub-sets of the complex plane 39, 47

ω If the inverse Laplace transform f does not satisfy

$$\lim_{t \to \infty} f(t) = 0,$$

then a function ω is determined in Section 1.4 such that $\omega(t) f(t)$ satisfies this condition 13

Upper case Greek letters

Γ Curve in the complex plane 2, 4, 39, 40, 45, 46

Δ Difference operator in (2.4.5) 31

Ω, Ω^* Subset of the complex plane 39, 42, 43, 44, 46

Ω_N Subset of the complex plane, consisting of N points 43

Other symbols

$\Re$ Real part of complex number 2, 7

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