

NUMERICAL ALGORITHMS

NUMERICAL METHODS FOR LAPLACE TRANSFORM INVERSION

ALAN M. COHEN

NUMERICAL METHODS FOR LAPLACE TRANSFORM INVERSION

Numerical Methods and Algorithms

VOLUME 5

Series Editor:

Claude Brezinski

Université des Sciences et Technologies de Lille, France

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Library of Congress Control Number: 2006940349

ISBN-13: 978-0-387-28261-9 e-ISBN-13: 978-0-387-68855-8

Printed on acid-free paper.

AMS Subject Classifications: 44A10, 44-04, 65D30, 65D32, 65Bxx

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Printed in the United States of America.

9 8 7 6 5 4 3 2 1

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Preface

The Laplace transform, as its name implies, can be traced back to the work of the Marquis Pierre-Simon de Laplace (1749-1827). Strange as it may seem no reference is made to Laplace transforms in Rouse Ball's "A Short Account of the History of Mathematics". Rouse Ball does refer to Laplace's contribution to Probability Theory and his use of the generating function. Nowadays it is well-known that if $\phi(t)$ is the probability density in the distribution function of the variate t , where $0 \leq t < \infty$, then the expected value of e^{st} is the Moment Generating Function which is defined by

$$M(s) = \int_0^{\infty} e^{st} \phi(t) dt. \quad (1)$$

The term on the right hand side of (1) is, if we replace s by $-s$, the quantity that we now call the Laplace transform of the function $\phi(t)$.

One of the earliest workers in the field of Laplace transforms was J.M. Petzval (1807-1891) although he is best remembered for his work on optical lenses and aberration which paved the way for the construction of modern cameras. Petzval [167] wrote a two volume treatise on the Laplace transform and its application to ordinary linear differential equations. Because of this substantial contribution the Laplace transform might well have been called the Petzval transform had not one of his students fallen out with him and accused him of plagiarising Laplace's work. Although the allegations were untrue it influenced Boole and Poincarè to call the transformation the Laplace transform.

The full potential of the Laplace transform was not realised until Oliver Heaviside (1850-1925) used his operational calculus to solve problems in electromagnetic theory. Heaviside's transform was a multiple of the Laplace transform and, given a transform, he devised various rules for finding the original function but without much concern for rigour. If we consider the simple differential equation

$$\frac{d^2 y}{dt^2} + y = 1, \quad t > 0$$

with initial conditions $y(0) = y'(0) = 0$ then Heaviside would write py for dy/dt , $p^2 y$ for $d^2 y/dt^2$ and so on. Thus the given equation is equivalent to

$$(p^2 + 1)y = 1,$$

and the 'operational solution' is

$$y \equiv \frac{1}{p^2 + 1}.$$

Expanding the right hand side in powers of $1/p$ we obtain

$$y \equiv \frac{1}{p^2} - \frac{1}{p^4} + \frac{1}{p^6} - \dots$$

Heaviside regarded $1/p$ as equivalent to $\int_0^t 1 dt$, i.e. t , $1/p^2$ as $\int_0^t t dt = t^2/2!$, etc., so that the solution of the given differential equation is

$$y = \frac{t^2}{2!} - \frac{t^4}{4!} + \frac{t^6}{6!} - \cdots,$$

which is readily identified with $1 - \cos t$, the correct solution.

For a differential equation of the form (again using the notation $py = dy/dt$, etc.)

$$(a_0 p^n + a_1 p^{n-1} + \cdots + a_{n-1} p + a_n) y = 1,$$

satisfying

$$\left. \frac{d^r y}{dt^r} \right|_{t=0} = 0, \quad r = 0, 1, \cdots, n-1$$

Heaviside has the operational solution

$$y = \frac{1}{\phi(p)},$$

where we denote the n th degree polynomial by $\phi(p)$. If all the roots p_r , $r = 1, \cdots, n$ of the n th degree algebraic equation $\phi(p) = 0$ are distinct Heaviside gave the formula (known as the ‘Expansion Theorem’)

$$y = \frac{1}{\phi(0)} + \sum_{r=0}^n \frac{e^{p_r t}}{p_r \phi'(p_r)}. \quad (2)$$

Compare this to (1.23). Carslaw and Jaeger [31] give examples of Heaviside’s approach to solving partial differential equations where his approach is very haphazard. Curiously, in his obituaries, there is no reference to his pioneering work in the Operational Calculus.

Bateman (1882-1944) seems to have been the first to apply the Laplace transform to solve integral equations in the early part of the 20th century. Based on notes left by Bateman, Erdélyi [78] compiled a table of integral transforms which contains many Laplace transforms.

Bromwich (1875-1929), by resorting to the theory of functions of a complex variable helped to justify Heaviside’s methods to some extent and lay a firm foundation for operational methods. For the example given above he recognized that the solution of the second order equation could be expressed as

$$y = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{pt} \frac{dp}{p(p^2+1)},$$

where $\gamma > 0$. For the more general n th order equation we have

$$y = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{pt} \frac{dp}{p\phi(p)}, \quad (3)$$

where all the roots of $\phi(p) = 0$ lie to the left of $\Re p = \gamma$. The integral can be replaced by

$$y = \frac{1}{2\pi i} \int_{\mathcal{C}} e^{pt} \frac{dp}{p\phi(p)}, \quad (4)$$

where \mathcal{C} is any circular path with centre the origin which contains all the zeros of $\phi(p) = 0$ inside its circumference. Applying the Cauchy residue theorem to this integral leads to the expansion theorem (2). Again no specific mention of his contribution to the Operational Calculus was made in Bromwich's obituary (Hardy [111]). However, Jeffreys [118] gives an exposition of his methods in his book.

Starting in the 1920's considerable effort was put into research on transforms. In particular, Carson [32] and van der Pol made significant contributions to the study of Heaviside transforms. Thus Carson established, for the differential equation considered above, that

$$\frac{1}{\phi(p)} = p \int_0^\infty e^{-pt} y(t) dt. \quad (5)$$

Van der Pol gave a simpler proof of Carson's formula and showed how it could be extended to deal with non-zero initial conditions. Doetsch in his substantial contributions to transform theory preferred to use the definition that is now familiar as the Laplace transform

$$\bar{f}(s) = \int_0^\infty e^{-st} f(t) dt. \quad (6)$$

Another researcher who made significant contributions to the theory of Laplace transforms was Widder and in his book [253] he gives an exposition of the theory of the Laplace-Stieltjes transform

$$\bar{f}(s) = \int_0^\infty e^{-st} d\alpha(t), \quad (7)$$

where the function $\alpha(t)$ is of bounded variation in the interval $0 \leq t \leq R$ and the improper integral is defined by

$$\int_0^\infty e^{-st} d\alpha(t) = \lim_{R \rightarrow \infty} \int_0^R e^{-st} d\alpha(t).$$

This, of course, reduces to the standard definition of the Laplace transform when $d\alpha(t) = f(t)dt$ and $f(t)$ is a continuous function. An advantage of the Laplace-Stieltjes approach is that it enables us to deal in a sensible manner with functions of t which have discontinuities. In particular, we note that the inversion theorem takes the form (2.14) at a point of discontinuity.

Many other mathematicians made contributions to the theory of Laplace transforms and we shall just recall Tricomi [233] who used expansions in terms of Laguerre polynomials in order to facilitate the inversion of Laplace transforms.

The reader should consult Widder and the references therein for more details. Also quite a number of reference works appeared with tables of functions and their Laplace transforms, e.g. Roberts and Kaufman [197] — nearly all these results having been found painstakingly by contour integration methods.

With the advent of computers an opportunity arose to find out if one could develop methods which would produce accurate numerical answers for the inverse Laplace transform. A great deal has been achieved and this book gives some insight into the State of the Art. When a function has an explicit Laplace transform which has no poles to the right of $\Re s = c (c > 0)$ and only a finite number of poles to the left then, at this juncture in time, it is reasonable to expect that $f(t)$ can be computed to a high degree of accuracy for moderate values of t . When $f(s)$ has an infinity of poles on the imaginary axis then matters are not quite so straightforward and results can be very unreliable. Clearly this is an area where further research would be worthwhile. Where $\bar{f}(s)$ is determined by numerical values we again cannot expect to obtain accurate results. In many cases we have to rely on ad hoc methods such as interpolation or least squares to re-construct the function (see Applications §10.1 and §10.3) and, in general, we cannot expect good results unless, as in §10.1, we can compute $\bar{f}(s)$ very accurately. A blossoming area of current research is to find reliable techniques for the inversion of multidimensional transforms and a brief account has been given in the text.

This book is divided into a number of parts. The Preface gives a brief historical introduction. Chapters 1 and 2 provide basic theory. Chapters 3 - 8 outline methods that have been developed to find $f(t)$ for given t and $\bar{f}(s)$. Chapter 9 presents the conclusions of various surveys which have been carried out on the efficacies of these methods. In Chapter 10 we give some case studies of Applications. Chapter 11 gives background material needed to understand the methods discussed in earlier chapters. Readers can access a selection of FORTRAN and Mathematica programs of some of the most efficient numerical techniques from the website www.cf.ac.uk/maths/cohen/programs/inverselaplace transform/. When using these programs the user should try at least two different methods to confirm agreement of the numerical results as, occasionally, one method may fail for no accountable reason or it may be that t is too large or there has been severe cancellation of terms involved in the methods.

It is hoped that this book will be a useful tool for all those who use Laplace transforms in their work whether they are engineers, financial planners, mathematicians, scientists or statisticians. The book can also be used to provide a balanced course on Laplace transforms consisting of theory, numerical techniques and Applications.

Acknowledgements

My interest in Numerical Methods for Laplace Transform Inversion was kindled by a chance meeting with the late Professor Ivor Longman at a Conference in London about 30 years ago. As a result I became involved in developing methods for quadrature and series summation — fields in which Ivor’s former students Professors David Levin and Avraham Sidi are leading figures. I would like to thank them and also Professors David Evans ¹ and Gwynne Evans for their encouragement and support over the years. My colleagues in Mathematics and Computing at Cardiff University have also given me a great deal of help with checking theorems, writing/running computer programs and sorting out my problems with L^AT_EX. Any errors remaining, as well as any omissions, are due solely to me. I would also like to take this opportunity to thank all my former students and teachers. While I am unable to gauge how much I learnt from each of these groups, there is a saying in the Talmud which puts it in a nutshell. “From my teachers have I learnt much, from my colleagues more, but from my students have I learnt most”.

I am particularly grateful to the Vice-Chancellor of Cardiff University for granting me a Sabbatical during which I was able to complete several Chapters of the book. I would like to thank the Springer reviewers for their constructive criticisms of my first draft which have improved the content and presentation of the work. Also, thanks are due to the series editor Professor Claude Brezinski for his helpful comments which led to further improvements. Finally, my thanks to John Martindale and Robert Saley and their team at Springer for their patience and encouragement throughout the writing and revision.

¹Regrettably David passed away before this work was published.

Notation

i	$\sqrt{(-1)}$
$f^{(n)}(t)$	n th derivative of $f(t)$
$\mathcal{L}\{f(t)\}$	Laplace transform of $f(t)$
$\bar{f}(s)$	$\mathcal{L}\{f(t)\}$
$\tilde{f}(t)$	numerical approximation to $f(t)$
$\mathcal{L}_2\{f(t_1, t_2)\}$	Laplace transform of $f(t_1, t_2)$
\mathcal{L}_C	Laplace-Carson transform
$\mathcal{L}^{-1}\{\bar{f}(s)\}$	inverse transform of $\bar{f}(s)$
$\mathcal{L}_2^{-1}\{f(s_1, s_2)\}$	inverse transform of $\bar{f}(s_1, s_2)$
s	parameter in the Laplace transformation
$\Re s$	real part of s
$\Im s$	imaginary part of s
γ	smallest real part of s for which Laplace transform is convergent
c	real number $\geq \gamma$
$\mathcal{Z}\{f(t)\}$	z – transform of $f(t)$
$\mathfrak{B}, \mathfrak{B}', \mathcal{C}$	integration path
\mathfrak{F}	Fourier transform
\mathfrak{F}_C	Fourier cosine transform
\mathfrak{F}_S	Fourier sine transform
$H(t)$	Heaviside unit step function
$\delta(t)$	unit impulse function
$\operatorname{erf}(x)$	the error function
$E_1(x)$	the exponential integral
$\Gamma(x)$	the gamma function
$n!$	factorial function
$(n)_i$	Pochhammer symbol
$\psi(n)$	Psi or Digamma function
C	Euler's constant
$T_n(x)$	Chebyshev polynomial of first kind
$T_n * (x)$	shifted Chebyshev polynomial of first kind
$U_n(x)$	Chebyshev polynomial of second kind
$P_n(x)$	Legendre polynomial
$L_n(x)$	Laguerre polynomial
$\Phi_n(x)$	orthogonal Laguerre function

$L^{(n)}(x)$	n -point Lagrange interpolation polynomial
$J_n(t)$	n th order Bessel function
$I_n(t)$	n th order modified Bessel function
$\text{Ci}(t)$	cosine integral
$\text{Si}(t)$	sine integral
$C(t), S(t)$	Fresnel integrals
$M(a, b, z)$	Kummer confluent hypergeometric function
Δ	forward difference operator
$[x]$	integer part of x
\hat{z}	complex conjugate of z
$f[x_0, x_1, \dots, x_r]$	r th divided difference
$[p/q]$	notation for Padé approximant
$\text{sgn}(x)$	sign of x
$\ \dots\ $	an appropriate norm
$\langle \cdot, \cdot \rangle$	vector inner product

Chapter 1

Basic Results

1.1 Introduction

The principal object of this work is to bring together in one volume details of the various methods which have been devised for the numerical inversion of Laplace Transforms and to try and give some indication of how effective these methods are. In order to understand these methods we need to be familiar with basic results about Laplace transforms and these are presented in this and the next chapter.

Definition 1.1 The Laplace transform of the function $f(t)$ is defined by

$$\mathcal{L}\{f(t)\} = \int_0^{\infty} e^{-st} f(t) dt. \quad (1.1)$$

In general, we shall denote the transform by $\bar{f}(s)$. We assume that in (1.1) the function $f(t)$ is defined for all positive t in the range $(0, \infty)$, s is real and, most importantly, that the integral is convergent. A necessary condition for convergence is that

$$\Re s > \gamma, \quad \text{where } \gamma \text{ is a constant,}$$

and $f(t)$ satisfies

$$|f(t)| = O(e^{\gamma t}) \quad \text{as } t \rightarrow \infty. \quad (1.2)$$

This condition implies that the function $f(t)$ is smaller in magnitude than the term e^{-st} for large t ($> t_0$, say) and, unless $f(t)$ has some singularity for $t < t_0$, the integral in (1.1) is convergent. Additionally, we can infer that

$$\bar{f}(s) \rightarrow 0, \quad \text{as } s \rightarrow \infty.$$

A most important consequence of the above is that $\bar{f}(s)$ will be an analytic function in the half-plane $\Re s > \gamma$, a result which will have application in subsequent chapters.

Because of the restrictions imposed by (1.2) it is clear that a function such as $\exp(t^2)$ cannot have a Laplace transform since no value of the constant γ can be found for which

$$|e^{t^2}| < e^{\gamma t},$$

for large t . The restriction that $f(t)$ should be continuous can be relaxed and later we shall determine the Laplace transforms of functions which are periodic, with period T , and which have an infinite number of discontinuities.

1.2 Transforms of Elementary Functions

Integration yields

$$\begin{aligned}\mathcal{L}\{1\} &= \int_0^\infty e^{-st} dt = 1/s, \quad (s > 0). \\ \mathcal{L}\{t\} &= \int_0^\infty e^{-st} t dt = \left(\frac{-te^{-st}}{s} \right) \Big|_0^\infty + \int_0^\infty (e^{-st}/s) dt, \\ &= (1/s) \int_0^\infty e^{-st} dt = 1/s^2,\end{aligned}$$

If we let

$$I_n = \int_0^\infty e^{-st} t^n dt, \quad (n \text{ an integer})$$

then, by integration by parts, we find

$$I_n = (n/s) I_{n-1}.$$

Repeated application of this result yields

$$\mathcal{L}\{t^n\} = I_n = (n/s) I_{n-1} = \cdots = (n!/s^n) I_0 = n!/s^{n+1}.$$

Also

$$\mathcal{L}\{e^{\alpha t}\} = \int_0^\infty e^{-st} e^{\alpha t} dt = \int_0^\infty e^{-(s-\alpha)t} dt = 1/(s-\alpha).$$

The integral converges provided that $\Re s > \alpha$. Again

$$\mathcal{L}\{\sin \omega t\} = \int_0^\infty e^{-st} \sin \omega t dt = I, \quad \text{say.}$$

Integration by parts produces

$$\begin{aligned}I &= -\frac{1}{\omega} \cos \omega t e^{-st} \Big|_0^\infty - \frac{s}{\omega} \int_0^\infty e^{-st} \cos \omega t dt, \\ &= \frac{1}{\omega} - \frac{s}{\omega} \left\{ \frac{1}{\omega} e^{-st} \sin \omega t \Big|_0^\infty + \frac{s}{\omega} \int_0^\infty e^{-st} \sin \omega t dt \right\}.\end{aligned}$$

Thus

$$I = \frac{1}{\omega} - \frac{s^2}{\omega^2} I,$$

which, after rearrangement, gives

$$\mathcal{L}\{\sin \omega t\} = I = \omega/(s^2 + \omega^2).$$

Similarly,

$$\mathcal{L}\{\cos \omega t\} = s/(s^2 + \omega^2).$$

A list of the more useful transforms is given in Appendix 11.1.

1.2.1 Elementary Properties of Transforms

It follows from (1.1) that if $f(t)$ and $g(t)$ are any two functions satisfying the conditions of the definition then

$$\begin{aligned} \mathcal{L}\{f(t) + g(t)\} &= \int_0^\infty e^{-st}(f(t) + g(t))dt, \\ &= \int_0^\infty e^{-st}f(t)dt + \int_0^\infty e^{-st}g(t)dt, \end{aligned}$$

i.e.

$$\mathcal{L}\{f(t) + g(t)\} = \bar{f}(s) + \bar{g}(s). \quad (1.3)$$

Also

$$\begin{aligned} \mathcal{L}\{\kappa f(t)\} &= \int_0^\infty e^{-st}(\kappa f(t))dt, \quad \kappa \text{ a constant} \\ &= \kappa \int_0^\infty e^{-st}f(t)dt, \end{aligned}$$

i.e.

$$\mathcal{L}\{\kappa f(t)\} = \kappa \bar{f}(s). \quad (1.4)$$

From (1.3) and (1.4) and the results of the previous section we can determine the Laplace transforms of any linear combination of the functions 1, t^n , $e^{\alpha t}$, $\sin \omega t$ and $\cos \omega t$. For example,

$$\begin{aligned} \mathcal{L}\{3 + t^2 + 2e^{-t} + \sin 2t\} &= \mathcal{L}\{3\} + \mathcal{L}\{t^2\} + \mathcal{L}\{2e^{-t}\} + \mathcal{L}\{\sin 2t\}, \\ &= \frac{3}{s} + \frac{2}{s^3} + \frac{2}{s+1} + \frac{2}{s^2 + 4}. \end{aligned}$$

In some instances $\mathcal{L}\{f(t)\}$ will be known and it will be required to determine $\mathcal{L}\{f(at)\}$. We find, by making a change of variable in the defining relationship (1.1), that

$$\mathcal{L}\{f(at)\} = \frac{1}{a} \bar{f}\left(\frac{s}{a}\right). \quad (1.5)$$

If we define the function $h(t)$ by

$$h(t) = f(t) + ig(t), \quad i = \sqrt{-1},$$

then

$$\mathcal{L}\{h(t)\} = \mathcal{L}\{f(t)\} + i\mathcal{L}\{g(t)\} = \bar{f}(s) + i\bar{g}(s). \quad (1.6)$$

In particular, when $f(t)$, $g(t)$ and s are real

$$\left. \begin{aligned} \Re \mathcal{L}\{h(t)\} &= \bar{f}(s) \\ \Im \mathcal{L}\{h(t)\} &= \bar{g}(s) \end{aligned} \right\}. \quad (1.7)$$

Further, if $f(t)$ is a function with known transform $\bar{f}(s)$, it follows from (1.1) that

$$\begin{aligned} \mathcal{L}\{e^{-\alpha t} f(t)\} &= \int_0^\infty e^{-st} (e^{-\alpha t} f(t)) dt, \\ &= \int_0^\infty e^{-(s+\alpha)t} f(t) dt, \end{aligned}$$

and, by comparing the right hand side with (1.1), it is clear this represents a ‘transform’ having parameter $s + \alpha$. Thus we have the result

$$\mathcal{L}\{e^{-\alpha t} f(t)\} = \bar{f}(s + \alpha). \quad (1.8)$$

(1.8) is referred to as the *Shift theorem* for Laplace transforms although Doetsch [70] refers to it as the *damping theorem*. It follows from the Shift theorem that

$$\begin{aligned} \mathcal{L}\{te^{-\alpha t}\} &= 1/(s + \alpha)^2, \\ \mathcal{L}\{e^{-\alpha t} \sin \omega t\} &= \frac{\omega}{(s + \alpha)^2 + \omega^2}, \\ \mathcal{L}\{e^{-\alpha t} \cos \omega t\} &= \frac{s + \alpha}{(s + \alpha)^2 + \omega^2}. \end{aligned}$$

Since $e^{-i\omega t} = \cos \omega t - i \sin \omega t$ it follows from the Shift theorem and (1.6) that

$$\mathcal{L}\{f(t) \cos \omega t\} = \Re \bar{f}(s + i\omega), \quad (1.9)$$

$$\mathcal{L}\{f(t) \sin \omega t\} = -\Im \bar{f}(s + i\omega). \quad (1.10)$$

Another useful result is

$$\mathcal{L}\{tf(t)\} = -\frac{d}{ds}(\bar{f}(s)). \quad (1.11)$$

This result is valid whenever it is permissible to differentiate (1.1) under the sign of integration. We find by taking $f(t) = \cos \omega t$ that (1.11) yields

$$\mathcal{L}\{t \cos \omega t\} = \frac{s^2 - \omega^2}{(s^2 + \omega^2)^2},$$

a result which could also have been obtained by taking $f(t) = t$ in (1.9). Finally, in this section, we establish the result

$$\mathcal{L}\{f(t)/t\} = \int_s^\infty \bar{f}(v)dv. \quad (1.12)$$

The right hand side may be written as

$$\int_s^\infty \bar{f}(v)dv = \int_s^\infty \left(\int_0^\infty e^{-vt} f(t)dt \right) dv.$$

Assuming uniform convergence of the integrals the order of integration may be inverted and we have

$$\begin{aligned} \int_s^\infty \bar{f}(v)dv &= \int_0^\infty f(t) \left(\int_s^\infty e^{-vt} dv \right) dt, \\ &= \int_0^\infty f(t) \frac{e^{-st}}{t} dt = \int_0^\infty e^{-st} \left(\frac{f(t)}{t} \right) dt, \\ &= \mathcal{L}\{f(t)/t\}. \end{aligned}$$

It follows from (1.12) that

$$\begin{aligned} \mathcal{L}\left\{\frac{\sin t}{t}\right\} &= \int_s^\infty \frac{dv}{v^2 + 1} = \tan^{-1} v \Big|_s^\infty, \\ &= \frac{\pi}{2} - \tan^{-1} s. \end{aligned} \quad (1.13)$$

Note that it follows from (1.13), by taking $s = 0$ and $s = 1$ respectively, that

$$\int_0^\infty \frac{\sin t}{t} dt = \frac{\pi}{2},$$

and

$$\int_0^\infty \frac{e^{-t} \sin t}{t} dt = \frac{\pi}{4}.$$

1.3 Transforms of Derivatives and Integrals

In some of the most important applications of Laplace transforms we need to find the transform of $f'(t)$, the derivative of $f(t)$, higher derivatives of $f(t)$, and also $\int_0^t f(u)du$. Assume that $f(t)$ is differentiable and continuous and $O(e^{\gamma t})$ as $t \rightarrow \infty$. Further, $f'(t)$ is continuous except at a finite number of points t_1, t_2, \dots, t_n in any finite interval $[0, T]$. Then

$$\int_0^T e^{-st} f'(t)dt = \int_0^{t_1} e^{-st} f'(t)dt + \int_{t_1}^{t_2} e^{-st} f'(t)dt + \dots + \int_{t_n}^T e^{-st} f'(t)dt.$$

Integrating by parts a typical term on the right hand side is

$$\begin{aligned} \int_{t_r}^{t_{r+1}} e^{-st} f'(t) dt &= e^{-st} f(t) \Big|_{t_r}^{t_{r+1}} + s \int_{t_r}^{t_{r+1}} e^{-st} f(t) dt, \\ &= e^{-st_{r+1}} f(t_{r+1}-) - e^{-st_r} f(t_r+) + s \int_{t_r}^{t_{r+1}} e^{-st} f(t) dt, \end{aligned}$$

where

$$\begin{aligned} f(a-) &= \lim_{\epsilon \rightarrow 0} f(a - \epsilon), \\ f(a+) &= \lim_{\epsilon \rightarrow 0} f(a + \epsilon), \end{aligned}$$

and $\epsilon > 0$. Since $f(t)$ is continuous at each t_i we find

$$\int_0^T e^{-st} f'(t) dt = e^{-sT} f(T) - f(0+) + s \int_0^T e^{-st} f(t) dt.$$

Letting $T \rightarrow \infty$ we obtain the result

$$\mathcal{L}\{f'(t)\} = s\bar{f}(s) - f(0+). \quad (1.14)$$

If we assume that $f'(t)$ is continuous and differentiable and $f''(t)$ is continuous except at a finite number of points in any finite interval $(0, T)$ then

$$\mathcal{L}\{f''(t)\} = \mathcal{L}\left\{\frac{d}{dt}f'(t)\right\} = s\mathcal{L}\{f'(t)\} - f'(0+),$$

giving

$$\mathcal{L}\{f''(t)\} = s^2\bar{f}(s) - sf(0+) - f'(0+). \quad (1.15)$$

This result can be extended to higher derivatives to yield

$$\mathcal{L}\{f^{(n)}(t)\} = s^n\bar{f}(s) - s^{n-1}f(0+) - s^{n-2}f'(0+) - \dots - f^{(n-1)}(0+). \quad (1.16)$$

In most of the applications that we are interested in the function and its derivatives are continuous at $t = 0$ so that $f^{(n)}(0+)$ can be replaced by $f^{(n)}(0)$.

Another useful result is

$$\mathcal{L}\left\{\int_0^t f(u) du\right\} = \bar{f}(s)/s. \quad (1.17)$$

From the definition we have

$$\begin{aligned} \mathcal{L}\left\{\int_0^t f(u) du\right\} &= \int_0^\infty e^{-st} \left(\int_0^t f(u) du\right) dt, \\ &= -\frac{e^{-st}}{s} \left(\int_0^t f(u) du\right) \Big|_0^\infty + \int_0^\infty \frac{e^{-st}}{s} f(t) dt, \end{aligned}$$

by integrating by parts. Because we require the Laplace transform to be convergent it follows that $\int_0^t f(u)du$ must be majorised by e^{-st} as $t \rightarrow \infty$. At the lower limit the integrand is zero. Thus

$$\mathcal{L}\left\{\int_0^t f(u)du\right\} = \frac{1}{s} \int_0^\infty e^{-st} f(t)dt = \bar{f}(s)/s,$$

as required. Finally, in this section, we shall demonstrate how we can find the formal solution of a linear ordinary differential equation with constant coefficients.

Example 1.1 Solve the linear second order differential equation system

$$\frac{d^2 y}{dt^2} + \omega^2 y = 1, \quad y(0) = a, \quad y'(0) = b, \quad (1.18)$$

where $\omega(> 0)$, a and b are constants.

We can proceed in the following way. If $\bar{y}(s)$ is the Laplace transform of $y(t)$ it follows from (1.15) that

$$\mathcal{L}\left\{\frac{d^2 y}{dt^2}\right\} = s^2 \bar{y}(s) - sa - b,$$

and since $\mathcal{L}\{1\} = 1/s$ it follows that the Laplace transform of the differential equation is

$$s^2 \bar{y}(s) - sa - b + \omega^2 \bar{y}(s) = 1/s.$$

Collecting terms in $\bar{y}(s)$ this gives

$$(s^2 + \omega^2) \bar{y}(s) = sa + b + 1/s,$$

i.e.

$$\bar{y}(s) = \frac{sa + b}{s^2 + \omega^2} + \frac{1}{s(s^2 + \omega^2)},$$

and, by resolving into partial fractions, we obtain

$$\bar{y}(s) = \left(a - \frac{1}{\omega^2}\right) \frac{s}{s^2 + \omega^2} + \frac{b}{\omega} \frac{\omega}{s^2 + \omega^2} + \frac{1}{\omega^2} \frac{1}{s}.$$

By reference to the Table of Transforms in Appendix 11.1 we can infer that the right hand side is the Laplace transform of

$$\left(a - \frac{1}{\omega^2}\right) \cos \omega t + \frac{b}{\omega} \sin \omega t + \frac{1}{\omega^2},$$

and we therefore assert that

$$y(t) = \left(a - \frac{1}{\omega^2}\right) \cos \omega t + \frac{b}{\omega} \sin \omega t + \frac{1}{\omega^2}, \quad (1.19)$$

is a solution of the differential equation system (1.18). Substitution of $y(t)$ in the differential equation and evaluation of $y(0)$ and $y'(0)$ confirms this.

1.4 Inverse Transforms

If $\mathcal{L}\{f(t)\} = \bar{f}(s)$ then we write $\mathcal{L}^{-1}\{\bar{f}(s)\}$ to denote the function whose Laplace transform is $\bar{f}(s)$. Thus

$$f(t) = \mathcal{L}^{-1}\{\bar{f}(s)\}, \quad (1.20)$$

and we say that $f(t)$ is the *inverse transform* of $\bar{f}(s)$. From the previous sections it is evident that

$$\mathcal{L}^{-1}\left\{\frac{1}{s^2}\right\} = t, \quad \mathcal{L}^{-1}\left\{\frac{s}{s^2 + \omega^2}\right\} = \cos \omega t.$$

It is not difficult to establish that if a function $f_1(t)$ differs from $f(t)$ only at a finite set of values t_1, t_2, \dots, t_n then

$$\mathcal{L}\{f_1(t)\} = \mathcal{L}\{f(t)\},$$

so that the inverse transform is not unique. As we shall see in the next chapter the Laplace transform is unique if $f(t)$ is continuous in the interval $[0, \infty)$. This condition will be tacitly assumed throughout the book unless otherwise stated. In the last section we found that we could solve a differential equation if it was possible to express a rational function of s in terms of functions whose inverse transforms were known. More generally, if

$$\bar{f}(s) = P(s)/Q(s), \quad \deg P < \deg Q, \quad (1.21)$$

and

$$Q(s) = (s - \alpha_1)(s - \alpha_2) \cdots (s - \alpha_n), \quad (1.22)$$

where the α_k are all distinct, then $\bar{f}(s)$ can be written as

$$\bar{f}(s) = \sum_{k=1}^n \frac{P(\alpha_k)}{(s - \alpha_k)Q'(\alpha_k)},$$

so that

$$\mathcal{L}^{-1}\{\bar{f}(s)\} = \sum_{k=1}^n \frac{P(\alpha_k)}{Q'(\alpha_k)} e^{\alpha_k t}. \quad (1.23)$$

This result is known as the *expansion theorem*. If one of the roots α_k is repeated m times then the expansion for $\bar{f}(s)$ contains terms of the form

$$\frac{A_1}{s - \alpha_k} + \frac{A_2}{(s - \alpha_k)^2} + \cdots + \frac{A_m}{(s - \alpha_k)^m},$$

where

$$A_{m-r} = \lim_{s \rightarrow \alpha_k} \left[\frac{1}{r!} \frac{d^r}{ds^r} ((s - \alpha_k)^m \bar{f}(s)) \right].$$

Example 1.2 Find $\mathcal{L}^{-1}\{1/s(s-1)^3\}$.

From the above it is clear that $\bar{f}(s)$ must have the form

$$\bar{f}(s) = \frac{A}{s} + \frac{B}{s-1} + \frac{C}{(s-1)^2} + \frac{D}{(s-1)^3}.$$

where

$$A = \lim_{s \rightarrow 0} 1/(s-1)^3 = -1,$$

$$B = \lim_{s \rightarrow 1} \frac{1}{2!} \frac{d^2}{ds^2} \frac{1}{s} = 1,$$

$$C = \lim_{s \rightarrow 1} \frac{d}{ds} \frac{1}{s} = -1,$$

$$D = \lim_{s \rightarrow 1} \frac{1}{s} = 1.$$

Thus

$$\bar{f}(s) = \frac{-1}{s} + \frac{1}{s-1} + \frac{-1}{(s-1)^2} + \frac{1}{(s-1)^3},$$

and

$$f(t) = \mathcal{L}^{-1}\{f(s)\} = -1 + e^t - te^t + \frac{1}{2}t^2e^t.$$

The same result could have been achieved by the equivalent method of *partial fractions*. In the next chapter we will show how the inverse transform of more general functions can be determined.

1.5 Convolution

Consider the following example which differs from Example 1.1 only in consequence of the right hand side of the differential equation not being given explicitly.

Example 1.3 Solve the linear second order ordinary differential equation system

$$\frac{d^2y}{dt^2} + \omega^2y = f(t), \quad y(0) = a, \quad y'(0) = b, \quad (1.24)$$

where $f(t)$ is a function of t to be specified and ω , a , b are constants.

Proceeding as in Example 1.1 we find that if $\bar{y} = \bar{y}(s) = \mathcal{L}\{y(t)\}$ and $\bar{f} = \bar{f}(s) = \mathcal{L}\{f(t)\}$ then the Laplace transform of the differential equation is

$$s^2\bar{y} - sa - b + \omega^2\bar{y} = \bar{f}.$$

Thus

$$\bar{y} = a \cdot \frac{s}{s^2 + \omega^2} + \left(\frac{b}{\omega}\right) \frac{\omega}{s^2 + \omega^2} + \left(\frac{1}{\omega}\right) \cdot \bar{f} \cdot \frac{\omega}{s^2 + \omega^2}.$$

Now the first term on the right hand side is clearly the transform of $a \cos \omega t$ and the second term is the transform of $(b/\omega) \sin \omega t$ but, without more precise

information about \bar{f} , we cannot deduce anything about the last term using our current knowledge of Laplace transforms. The following theorem enables us to give an explicit formula for the inverse transform of the final term. We have

Theorem 1.1 The Convolution Theorem. *If $\bar{f}_1(s)$ is the Laplace transform of $f_1(t)$ and $\bar{f}_2(s)$ is the Laplace transform of $f_2(t)$ then*

$$\mathcal{L}^{-1}\{\bar{f}_1(s)\bar{f}_2(s)\} = \int_0^t f_1(u)f_2(t-u)du, \quad (1.25)$$

— this theorem is sometimes referred to as the *Composition theorem* or the *Faltung theorem* or *Duhamel's theorem*. The integral on the right hand side of (1.25) is known as the convolution of $f(t)$ and $g(t)$ and is written as $(f * g)(t)$. *Proof.* Assume that the integrals defining $\bar{f}_1(s)$ and $\bar{f}_2(s)$ converge absolutely on $s = s_0 > 0$. Then we know that

$$\int_0^\infty e^{-s_0 u} f_1(u) du \int_0^\infty e^{-s_0 v} f_2(v) dv = \int \int e^{-s_0(u+v)} f_1(u) f_2(v) du dv,$$

where the double integral is taken over the quadrant $u > 0, v > 0$. The substitution $u = u, u + v = t$ transforms the double integral into

$$\int \int e^{-s_0 t} f_1(u) f_2(t-u) du dt,$$

taken over the region between the u -axis and the line $u = t$ in the u, t plane. This double integral is equal to the repeated integral

$$\int_0^\infty e^{-s_0 t} \left\{ \int_0^t f_1(u) f_2(t-u) du \right\} dt.$$

Since the absolute convergence for $s = s_0 > 0$ implies absolute convergence for $s > s_0$ we have established the theorem. ■

Applying the above theorem to the transform in the above example we find that the third term is the transform of

$$\frac{1}{\omega} \int_0^t f(u) \sin \omega(t-u) du,$$

and hence the complete solution of the differential equation system (1.24) is given for general $f(t)$ by

$$y(t) = a \cos \omega t + (b/\omega) \sin \omega t + (1/\omega) \int_0^t f(u) \sin \omega(t-u) du. \quad (1.26)$$

When $f(t)$ is specified then $y(t)$ can be determined explicitly by evaluating the integral in (1.26).

We remark that the Convolution theorem can be applied to solve Volterra integral equations of the first and second kind where the kernel is of convolution type.

Example 1.4 Solve the equation

$$\int_0^t \cos(t-x)\phi(x)dx = \sin t.$$

Taking Laplace transforms of both sides we have

$$\frac{s}{s^2+1}\bar{\phi}(s) = \frac{1}{s^2+1},$$

which implies that

$$\bar{\phi}(s) = \frac{1}{s},$$

i.e.

$$\phi(t) = 1.$$

With the general Volterra equation of the first kind

$$\int_0^t K(t-x)\phi(x)dx = g(t),$$

then

$$\bar{\phi}(s) = \bar{g}(s)[\bar{K}(s)]^{-1}.$$

Now $[\bar{K}(s)]^{-1}$ cannot be a Laplace transform since it does not tend to zero as $s \rightarrow \infty$. Hence, for $\phi(t)$ to exist as an ordinary function $g(t)$ must be a function which satisfies

$$\bar{g}(s)[\bar{K}(s)]^{-1} \rightarrow 0 \quad \text{as } |s| \rightarrow \infty.$$

1.6 The Laplace Transforms of some Special Functions

The Heaviside Unit Step Function

The discontinuous function $H(t)$ defined by

$$H(t) = \begin{cases} 0 & \text{when } t < 0 \\ 1 & \text{when } t > 0 \end{cases}, \quad (1.27)$$

is called the (Heaviside) unit step function. We have

$$\mathcal{L}\{H(t)\} = \int_0^\infty e^{-st}H(t)dt = \int_0^\infty e^{-st}dt = \frac{1}{s}.$$

Similarly,

$$H(t-a) = \begin{cases} 0 & \text{when } t < a \\ 1 & \text{when } t > a \end{cases}.$$

It therefore represents a unit step function applied at $t = a$. Its Laplace transform is given by

$$\begin{aligned} \mathcal{L}\{H(t-a)\} &= \int_0^\infty e^{-st} H(t-a) dt = \int_a^\infty e^{-st} H(t) dt, \\ &= \left[-\frac{e^{-st}}{s} \right]_a^\infty = \frac{e^{-as}}{s}. \end{aligned} \quad (1.28)$$

Note that a is always positive since $t = 0$ represents the start of observations. A particularly useful result involving the unit step function is

$$\mathcal{L}\{H(t-a)f(t-a)\} = e^{-as}\bar{f}(s). \quad (1.29)$$

This is referred to by Doetsch as the *translation theorem* and by Bellman and Roth as the *exponential shift theorem*.

The function

$$\kappa[H(t-a) - H(t-b)],$$

where $a < b$, is equal to 0 when $t < a$, κ when $a < t < b$ and 0 when $t > b$. It is called a pulse of duration $b-a$, magnitude κ and strength $\kappa(b-a)$. Its Laplace transform is

$$\kappa(e^{-as} - e^{-bs})/s.$$

The Unit Impulse Function

A pulse of large magnitude, short duration and finite strength is called an impulse. The unit impulse function, denoted by $\delta(t)$, and sometimes called the delta function, is an impulse of unit strength at $t = 0$. It is the limit of a pulse of duration α and magnitude $1/\alpha$ as $\alpha \rightarrow 0$. Thus

$$\delta(t) = \lim_{\alpha \rightarrow 0} \left\{ \frac{H(t) - H(t-\alpha)}{\alpha} \right\}. \quad (1.30)$$

It follows that

$$\mathcal{L}\{\delta(t)\} = \lim_{\alpha \rightarrow 0} \left(\frac{1 - e^{-\alpha s}}{\alpha s} \right),$$

and, applying l'Hôpital's rule,

$$\text{the right hand side} = \lim_{\alpha \rightarrow 0} \frac{se^{-\alpha s}}{s} = 1.$$

Thus

$$\mathcal{L}\{\delta(t)\} = 1. \quad (1.31)$$

The function $\delta(t - a)$ represents an unit impulse function applied at $t = a$. Its Laplace transform is given by

$$\mathcal{L}\{\delta(t - a)\} = e^{-as}.$$

The impulse function is useful when we are trying to model physical situations, such as the case of two billiard balls impinging, where we have a large force acting for a short time which produces a finite change of momentum.

Periodic functions

Sometimes, particularly in problems involving electrical circuits, we have to find the Laplace transform of a function $f(t)$ with the property that

$$f(t + T) = f(t), \quad t > 0. \quad (1.32)$$

where T is a constant. Such a function is called periodic and the most frequently occurring examples of periodic functions are $\cos t$ and $\sin t$. The Laplace transform of $f(t)$ is given by

$$\begin{aligned} \bar{f}(s) &= \int_0^{\infty} e^{-st} f(t) dt, \\ &= \int_0^T e^{-st} f(t) dt + \int_T^{2T} e^{-st} f(t) dt + \cdots + \int_{kT}^{(k+1)T} e^{-st} f(t) dt + \cdots. \end{aligned}$$

But

$$\int_{kT}^{(k+1)T} e^{-st} f(t) dt = e^{-ksT} \int_0^T e^{-st} f(t) dt,$$

which implies that

$$\bar{f}(s) = (1 + e^{-sT} + e^{-2sT} + \cdots + e^{-ksT} + \cdots) \int_0^T e^{-st} f(t) dt.$$

The geometric series has common ratio $e^{-sT} < 1$ for all real $s > \gamma$ and therefore it converges to $1/(1 - e^{-sT})$ giving

$$\mathcal{L}\{f(t)\} = \frac{\int_0^T e^{-st} f(t) dt}{1 - e^{-sT}}. \quad (1.33)$$

Example 1.5 Find the Laplace transform of the Square Wave function

$$f(t) = \begin{cases} 1, & 0 < t < \frac{1}{2}T \\ -1, & \frac{1}{2}T < t < T \end{cases}. \quad (1.34)$$

Applying the result (1.33) we have

$$\begin{aligned}
 \bar{f}(s) &= \left(\int_0^{\frac{1}{2}T} e^{-st} dt - \int_{\frac{1}{2}T}^T e^{-st} dt \right) / (1 - e^{-sT}), \\
 &= \left(\frac{1 - 2e^{-\frac{1}{2}sT} + e^{-sT}}{s} \right) / (1 - e^{-sT}), \\
 &= \frac{1 - e^{-\frac{1}{2}sT}}{s(1 + e^{-\frac{1}{2}sT})}, \\
 &= \frac{1}{s} \tanh \frac{1}{4}sT.
 \end{aligned}$$

A comprehensive list of transforms can be found in Roberts and Kaufman [197] and Erdélyi [78], for example. A selected list of transforms is given in Appendix 11.1.

1.7 Difference Equations and Delay Differential Equations

We have seen that linear ordinary differential equations and convolution type Volterra integral equations can be solved by means of Laplace transforms. Another type of problem which is amenable to solution by Laplace transforms is that of difference equations. Suppose we are given a_0 . Define $y(t) = a_n$ for $n \leq t < n+1$ where $n = 0, 1, 2, \dots$. Then, if $\bar{y}(s) = \mathcal{L}\{y(t)\}$, we have

$$\begin{aligned}
 \mathcal{L}\{y(t+1)\} &= \int_0^\infty e^{-st} y(t+1) dt, \\
 &= \int_1^\infty e^{-s(u-1)} y(u) du, \\
 &= e^s \left[\int_0^\infty e^{-su} y(u) du - \int_0^1 e^{-su} y(u) du \right], \\
 &= e^s \left[y(s) - \int_0^1 e^{-su} a_0 du \right], \\
 &= e^s \bar{y}(s) - \frac{a_0 e^s (1 - e^{-s})}{s}.
 \end{aligned} \tag{1.35}$$

Similarly we can establish that

$$\mathcal{L}\{y(t+2)\} = e^{2s} \bar{y}(s) - \frac{e^s (1 - e^{-s})(a_0 e^s + a_1)}{s}. \tag{1.36}$$

We will now employ the above results to determine the solution of a difference equation.

Example 1.6 Solve the difference equation $a_{n+2} - 5a_{n+1} + 6a_n = 0$, $a_0 = 0$, $a_1 = 1$.

Write, as before, $y(t) = a_n$, $n \leq t < n + 1$. Then

$$y(t+2) - 5y(t+1) + 6y(t) = 0.$$

Taking Laplace transforms

$$e^{2s}\bar{y}(s) - \frac{e^s(1 - e^{-s})}{s} - 5e^s\bar{y}(s) + 6\bar{y}(s) = 0.$$

Collecting together the terms in $\bar{y}(s)$ and rearranging produces

$$\begin{aligned}\bar{y}(s) &= \frac{e^s(1 - e^{-s})}{s} \left[\frac{1}{(e^s - 3)(e^s - 2)} \right], \\ &= \frac{e^s(1 - e^{-s})}{s(e^s - 3)} - \frac{e^s(1 - e^{-s})}{s(e^s - 2)}.\end{aligned}$$

From Appendix 12.1, $\mathcal{L}\{f(t)\} = (1 - e^{-s})/s(1 - re^{-s})$ if $f(t) = r^n$, $n \leq t < n + 1$ and thus

$$y(t) = 3^{[t]} - 2^{[t]} \Rightarrow a_n = 3^n - 2^n,$$

where $[t]$ denotes the integer part of t .

We can also use the method of Laplace transforms to solve differential difference equations.

Example 1.7 Solve $y'(t) + y(t - 1) = t^2$ if $y(t) = 0$ for $t \leq 0$.

Taking the Laplace transform of both sides

$$\mathcal{L}\{y'(t)\} + \mathcal{L}\{y(t - 1)\} = 2/s^3.$$

Now

$$\mathcal{L}\{y'(t)\} = s\bar{y} - y(0) = s\bar{y},$$

and

$$\begin{aligned}\mathcal{L}\{y(t - 1)\} &= \int_0^\infty e^{-st}y(t - 1)dt, \\ &= \int_{-1}^\infty e^{-s(u+1)}y(u)du, \\ &= e^{-s} \left[\int_{-1}^0 e^{-su}y(u)du + \int_0^\infty e^{-su}y(u)du \right], \\ &= e^{-s}\bar{y}(s).\end{aligned}$$

Thus

$$s\bar{y} + e^{-s}\bar{y} = 2/s^3,$$

giving

$$\bar{y} = 2/s^3(s + e^{-s}).$$

We have

$$\begin{aligned}\bar{y} &= \frac{2}{s^4(1 + e^{-s}/s)}, \\ &= \frac{2}{s^4} \left(1 - \frac{e^{-s}}{s} + \frac{e^{-2s}}{s^2} - \dots \right), \\ &= \frac{2}{s^4} - \frac{2e^{-s}}{s^5} + \frac{2e^{-2s}}{s^6} - \dots, \\ &= 2 \sum_{n=0}^{\infty} (-1)^n \frac{e^{-ns}}{s^{n+4}}.\end{aligned}$$

Since

$$\mathcal{L}^{-1} \left\{ \frac{e^{-ns}}{s^{n+4}} \right\} = \frac{(t-n)^{n+3}}{(n+3)!} H(t-n),$$

we find

$$y(t) = 2 \sum_{n=0}^{\lfloor t \rfloor} (-1)^n \frac{(t-n)^{n+3}}{(n+3)!},$$

where $\lfloor t \rfloor$ = greatest integer $\leq t$.

1.7.1 z-Transforms

An alternative way of solving difference equations is via z -transforms. z -transforms have applications in digital filtering and signal processing and other practical problems (see Vich [244] and Brezinski [26]).

In signal processing we have the transformation of an input signal $f(t)$ into an output signal $h(t)$ by means of a system G called a digital filter. If f is known for all values of t we have a continuous signal but it may only be known at equally spaced values of t , $t_n = nT$, $n = 0, 1, \dots$ where T is the period, in which case we have a discrete signal.

The z -transform of a discrete signal is given by

$$\mathcal{Z}\{f(t)\} = F(z) = \sum_{n=0}^{\infty} f_n z^{-n}, \quad f_n = f(nT).$$

Corresponding to the input sequence f_n we have an output sequence h_n where $h_n = h(nT)$. The corresponding transfer function is

$$\mathcal{Z}\{h(t)\} = H(z) = \sum_{n=0}^{\infty} h_n z^{-n}.$$

The system G can be represented by its so-called transfer function $G(z)$ which satisfies

$$H(z) = G(z)F(z).$$

If

$$G(z) = \sum_0^{\infty} g_n z^{-n}$$

then

$$h_n = \sum_{k=0}^{\infty} f_k g_{n-k}, \quad n = 0, 1, \dots \quad (1.37)$$

Given $\{f_n\}$ and $\{h_n\}$ then (1.37) enables $\{g_n\}$ to be computed.

An alternative way of looking at the input signal is to consider the function $f(t)$ as being composed of a sum of impulse functions applied at nT , $n = 0, 1, \dots$, i.e.,

$$f(t) = f_0 \delta(t) + f_1 \delta(t - T) + \dots + f_n \delta(t - nT) + \dots$$

The Laplace transform of $f(t)$ is

$$\bar{f}(s) = f_0 + f_1 e^{-Ts} + \dots + f_n e^{-nTs} + \dots$$

and, if we write $z = e^{Ts}$, we obtain

$$\bar{f}(s) = f_0 + f_1 z^{-1} + \dots + f_n z^{-n} + \dots = F(z),$$

which establishes the connection between z-transforms and Laplace transforms. To close this section we give an example of how z-transforms can be used to solve a difference equation.

Example 1.8 Find the solution of the difference equation

$$a_{n+2} - 5a_{n+1} + 6a_n = 3n, \quad n \geq 2; \quad a_0 = 0, \quad a_1 = 1.$$

If we multiply the difference equation by z^{-n} and sum over n we get

$$z^2 \sum_{n=0}^{\infty} \frac{a_{n+2}}{z^{n+2}} - 5z \sum_{n=0}^{\infty} \frac{a_{n+1}}{z^{n+1}} + 6 \sum_{n=0}^{\infty} \frac{a_n}{z^n} = \sum_{n=0}^{\infty} \frac{3n}{z^n}.$$

Denoting $\sum_{n=0}^{\infty} a_n/z^n$ by $A(z)$ this can be expressed as

$$z^2 A(z) - a_0 z^2 - a_1 z - 5[zA(z) - a_0 z] + 6A(z) = \frac{3z}{(z-1)^2},$$

from Appendix §11.1. Substituting the values of a_0 and a_1 and rearranging we find

$$A(z) = \frac{3z}{(z-2)(z-3)(z-1)^2} + \frac{z}{(z-2)(z-3)},$$

which, after resolution into partial fractions, yields

$$A(z) = \frac{\frac{7}{4}z}{z-3} - \frac{4z}{z-2} + \frac{\frac{9}{4}z}{z-1} + \frac{\frac{3}{2}z}{(z-1)^2}.$$

By reference to the table of z-transforms in §11.1 we find

$$a_n = \frac{7}{4}3^n - 4 \cdot 2^n + \frac{9}{4} + \frac{3}{2}n.$$

1.8 Multidimensional Laplace Transforms

We have restricted our exposition of Laplace transforms to functions of one variable but we could equally well extend our definition to a function of two or more variables. Thus if, for example, y is a function of the variables t_1, t_2 , i.e. $y = f(t_1, t_2)$ then we define

$$\mathcal{L}_2\{y\} = \bar{f}(s_1, s_2) = \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} f(t_1, t_2) dt_1 dt_2, \quad (1.38)$$

where, for convergence of the integrals, we have to impose restrictions on f and s_1, s_2 which are similar to those in §1.1, — see Ditkin and Prudnikov [67] for a fuller account of the criteria needed for convergence. We can, as earlier, deduce the Laplace transform for elementary functions of two variables. Useful general results are:-

1. If $f(t_1, t_2) = f_1(t_1)f_2(t_2)$ and $\mathcal{L}\{f_1(t_1)\} = \bar{f}_1(s_1)$ and $\mathcal{L}\{f_2(t_2)\} = \bar{f}_2(s_2)$ then

$$\mathcal{L}_2\{f(t_1, t_2)\} = \bar{f}_1(s_1)\bar{f}_2(s_2). \quad (1.39)$$

2. If the integral (1.38) converges boundedly at the point (s'_1, s'_2) then it converges boundedly at all points (s_1, s_2) for which

$$\Re(s_1 - s'_1) > 0, \quad \Re(s_2 - s'_2) > 0.$$

3. If the function $\bar{f}(s_1, s_2)$ is analytic in the region \mathcal{D} which consists of the set of all points (s_1, s_2) for which the integral (1.38) is boundedly convergent then

$$\frac{\partial^{m+n}}{\partial s_1^m \partial s_2^n} \bar{f}(s_1, s_2) = (-1)^{m+n} \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} t_1^m t_2^n f(t_1, t_2) dt_1 dt_2, \quad (1.40)$$

or, equivalently,

$$\mathcal{L}_2\{t_1^m t_2^n f(t_1, t_2)\} = (-1)^{m+n} \frac{\partial^{m+n}}{\partial s_1^m \partial s_2^n} \bar{f}(s_1, s_2). \quad (1.40')$$

Example 1.9 If $f(t_1, t_2) = e^{\alpha t_1 + \beta t_2}$ (α, β real numbers), then

$$\begin{aligned} \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} e^{\alpha t_1 + \beta t_2} dt_1 dt_2 &= \int_0^\infty e^{-s_1 t_1} e^{\alpha t_1} dt_1 \times \int_0^\infty e^{-s_2 t_2} e^{\beta t_2} dt_2, \\ &= \frac{1}{(s_1 - \alpha)(s_2 - \beta)}. \end{aligned}$$

The region of convergence is $\Re s_1 > \alpha$, $\Re s_2 > \beta$.

Example 1.10 If

$$f(t_1, t_2) = \begin{cases} e^{t_1} & \text{for } t_1 \leq t_2, \\ e^{t_2} & \text{for } t_1 > t_2, \end{cases}$$

then

$$\begin{aligned}
& \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} f(t_1, t_2) dt_1 dt_2 \\
&= \int_0^\infty e^{-s_2 t_2} dt_2 \left\{ \int_0^{t_2} e^{-s_1 t_1} e^{t_1} dt_1 + \int_{t_2}^\infty e^{-s_1 t_1} e^{t_2} dt_1 \right\}, \\
&= \int_0^\infty e^{-s_2 t_2} dt_2 \left\{ \int_0^{t_2} e^{-t_1(s_1-1)} dt_1 + e^{t_2} \int_{t_2}^\infty e^{-s_1 t_1} dt_1 \right\}, \\
&= \int_0^\infty e^{-s_2 t_2} dt_2 \left\{ \frac{-e^{-t_1(s_1-1)}}{(s_1-1)} \Big|_0^{t_2} + e^{t_2} \left(\frac{-e^{-s_1 t_1}}{s_1} \right) \Big|_{t_2}^\infty \right\}, \\
&= \int_0^\infty e^{-s_2 t_2} \left[\left(\frac{-e^{-t_2(s_1-1)}}{(s_1-1)} + \frac{1}{(s_1-1)} \right) + e^{t_2} \left(\frac{e^{-s_1 t_2}}{s_1} \right) \right] dt_2, \\
&= \frac{-1}{(s_1 + s_2 - 1)(s_1 - 1)} + \frac{1}{s_2(s_1 - 1)} + \frac{1}{s_1(s_1 + s_2 - 1)},
\end{aligned}$$

which simplifies to yield

$$\mathcal{L}_2\{f(t_1, t_2)\} = \frac{s_1 + s_2}{s_1 s_2 (s_1 + s_2 - 1)}.$$

The region of convergence is shown in fig.1.1

We can establish many more results but just give a few samples below:-

$$\begin{aligned}
\mathcal{L}_2\{1\} &= \frac{1}{s_1 s_2}, \\
\mathcal{L}_2\{t_1^j t_2^k\} &= \frac{j!k!}{s_1^{j+1} s_2^{k+1}}, \\
\mathcal{L}_2\{e^{-\alpha t_1 - \beta t_2} y\} &= f(s_1 + \alpha, s_2 + \beta), \\
\mathcal{L}_2\{\sin t_1\} &= \frac{1}{s_2(s_1^2 + 1)}, \\
\mathcal{L}_2\{\cos t_1 \cos t_2\} &= \frac{s_1 s_2}{(s_1^2 + 1)(s_2^2 + 1)}, \\
\mathcal{L}_2\{\sin(t_1 + t_2)\} &= \frac{s_1 + s_2}{(s_1^2 + 1)(s_2^2 + 1)}, \quad \text{etc.}
\end{aligned}$$

The convolution concept can be extended to functions of two variables and Ditkin and Prudnikov give the result:-

Theorem 1.2 *The convolution theorem for functions of two variables.*
If, at the point (s_1, s_2) the integral

$$\bar{f}(s_1, s_2) = \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} f(t_1, t_2) dt_1 dt_2,$$

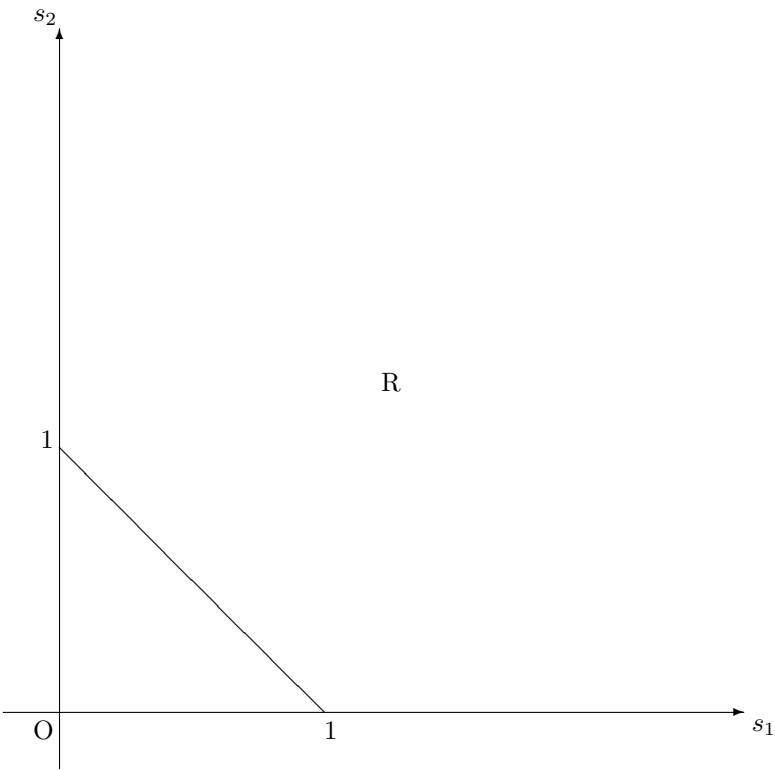


Figure 1.1: Region of convergence R

is boundedly convergent, and the integral

$$\bar{g}(s_1, s_2) = \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} g(t_1, t_2) dt_1 dt_2,$$

is absolutely convergent, then

$$\bar{h}(s_1, s_2) = \bar{f}(s_1, s_2) \bar{g}(s_1, s_2), \quad (1.41)$$

is the Laplace transform of the function

$$h(t_1, t_2) = \int_0^{t_1} \int_0^{t_2} f(t_1 - \xi_1, t_2 - \xi_2) g(\xi_1, \xi_2) d\xi_1 d\xi_2, \quad (1.42)$$

and the integral

$$\bar{h}(s_1, s_2) = \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} h(t_1, t_2) dt_1 dt_2,$$

is boundedly convergent at the point (s_1, s_2) . ■

Ditkin and Prudnikov find that there are some advantages in using the Laplace-Carson transform defined by

$$\mathcal{L}_C\{f(t_1, t_2)\} = \bar{f}_C(s_1, s_2) = s_1 s_2 \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} f(t_1, t_2) dt_1 dt_2. \quad (1.43)$$

This is essentially the two-dimensional analogue of the Heaviside transform and effectively $s_1 s_2$ times the Laplace transform \mathcal{L}_2 . With the above definition we have by integration by parts

$$\begin{aligned} s_1 \bar{f}_C(s_1, s_2) &= s_1 s_2 \int_0^\infty e^{-s_2 t_2} \left\{ -e^{-s_1 t_1} f(t_1, t_2) \Big|_{t_1=0}^\infty \right\} dt_2 \\ &\quad + s_1 s_2 \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} \frac{\partial f(t_1, t_2)}{\partial t_1} dt_1 dt_2, \\ &= s_1 s_2 \int_0^\infty e^{-s_2 t_2} f(0, t_2) dt_2 \\ &\quad + s_1 s_2 \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} \frac{\partial f(t_1, t_2)}{\partial t_1} dt_1 dt_2, \\ &= s_1 \mathcal{L}f(0, t_2) + \mathcal{L}_C \left\{ \frac{\partial f}{\partial t_1} \right\}. \end{aligned}$$

Thus

$$\mathcal{L}_C \left\{ \frac{\partial f}{\partial t_1} \right\} = s_1 [\bar{f}_C(s_1, s_2) - \mathcal{L}\{f(0, t_2)\}]. \quad (1.44)$$

Likewise we can establish

$$\mathcal{L}_C \left\{ \frac{\partial f}{\partial t_2} \right\} = s_2 [\bar{f}_C(s_1, s_2) - \mathcal{L}\{f(t_1, 0)\}]. \quad (1.45)$$

Other results which are easily deduced are:-

$$\mathcal{L}_C\{f(at_1, bt_2)\} = \bar{f}_C(s_1/a, s_2/b), \quad a, b > 0 \quad (1.46)$$

$$\mathcal{L}_C\{e^{-at_1-bt_2}f(t_1, t_2)\} = \frac{s_1 s_2}{(s_1 + a)(s_2 + b)} \bar{f}_C(s_1 + a, s_2 + b), \quad a, b \text{ arbitrary}, \quad (1.47)$$

$$\mathcal{L}_C\{g(t_1, t_2)\} = e^{-as_1-bs_2} \bar{g}_C(s_1, s_2), \quad (1.48)$$

where

$$g(t_1, t_2) = \begin{cases} 0 & t_1 < a \text{ or } t_2 < b \\ f(t_1 - a, t_2 - b) & t_1 > a, t_2 > b \end{cases}$$

More extensive results are given in Ditkin et al and we just quote here the result, where $L_n(x)$ denotes the Laguerre polynomial of degree n in the single variable x ,

$$\mathcal{L}_C\{e^{-t_1-t_2}L_n(t_1)L_n(t_2)\} = \left(\frac{s_1 s_2}{(1+s_1)(1+s_2)}\right)^{n+1}. \quad (1.49)$$

This, and similar results will be used in the 2-dimensional analogue of the Weeks' method (see Chapter 3).

Naturally, we can extend the definition to cover m variables so that if

$$y = f(t_1, t_2, \dots, t_m),$$

we have

$$\begin{aligned} \mathcal{L}_m\{y\} &= \bar{y}(s_1, \dots, s_m) \\ &= \underbrace{\int_0^\infty \dots \int_0^\infty}_m e^{-s_1 t_1 - \dots - s_m t_m} f(t_1, \dots, t_m) dt_1 \dots dt_m. \end{aligned} \quad (1.50)$$

More information on two dimensional Laplace transforms can be found in the works of van der Pol and Bremmer [240] or Voelker and Doetsch [245] and the Bibliography should be consulted, particularly in regard to numerical inversion.

Chapter 2

Inversion Formulae and Practical Results

2.1 The Uniqueness Property

We mentioned in the last Chapter that the Laplace transform is unique in the sense that if $\bar{f}(s) = \bar{g}(s)$ and $f(t)$ and $g(t)$ are continuous functions then $f(t) = g(t)$. This result was proved originally by Lerch [125] and the proof given here follows that in Carslaw and Jaeger [31].

Theorem 2.1 (*Lerch's theorem*).

If

$$\bar{f}(s) = \int_0^\infty e^{-st} f(t) dt, \quad s > \gamma, \quad (2.1)$$

is satisfied by a continuous function $f(t)$, there is no other continuous function which satisfies the equation (2.1).

Proof. We require the following lemma.

Lemma 2.1 Let $\psi(x)$ be a continuous function in $[0, 1]$ and let

$$\int_0^1 x^{n-1} \psi(x) dx = 0, \quad \text{for } n = 1, 2, \dots. \quad (2.2)$$

Then

$$\psi(x) \equiv 0, \quad \text{in } 0 \leq x \leq 1. \quad (2.3)$$

Proof. If $\psi(x)$ is not identically zero in the closed interval $[0, 1]$, there must be an interval $[a, b]$ where $0 < a < b < 1$ in which $\psi(x)$ is always positive (or always negative). We shall suppose the first alternative. By considering the function $(b-x)(x-a)$ we see that if

$$c = \max[ab, (1-a)(1-b)],$$

then

$$1 + \frac{1}{c}(b-x)(x-a) > 1, \quad \text{when } a < x < b$$

and

$$0 < 1 + \frac{1}{c}(b-x)(x-a) < 1, \quad \text{when } 0 < x < a \text{ and } b < x < 1.$$

Thus the function

$$p(x) = \{1 + (1/c)(b-x)(x-a)\}^r,$$

can be made as large as we please in $a < x < b$ and as small as we like in $0 < x < a$, $b < x < 1$ by appropriate choice of r . But $p(x)$ is a polynomial in x , and by our hypothesis

$$\int_0^1 x^{n-1} \psi(x) dx = 0, \quad \text{for } n = 1, 2, \dots$$

we should have

$$\int_0^1 p(x) \psi(x) dx = 0,$$

for every positive integer r . But the above inequalities imply that, by choosing r large enough,

$$\int_0^1 p(x) \psi(x) dx > 0.$$

The first alternative thus leads to a contradiction. A similar argument applies if we assume $\psi(x) < 0$ in (a, b) . It therefore follows that $\psi(x) \equiv 0$ in $[0, 1]$. ■

Now suppose that $g(t)$ is another continuous function satisfying (2.1) and define $h(t) = f(t) - g(t)$ which, as the difference of two continuous functions, is also continuous. Then

$$\int_0^\infty e^{-st} h(t) dt = 0, \quad s \geq \gamma. \quad (2.4)$$

Let $s = \gamma + n$, where n is any positive integer. Then

$$\begin{aligned} \int_0^\infty e^{-(\gamma+n)t} h(t) dt &= \int_0^\infty e^{-nt} (e^{-\gamma t} h(t)) dt, \\ &= \left[e^{-nt} \int_0^t e^{-\gamma u} h(u) du \right]_0^\infty + n \int_0^\infty e^{-nt} \left[\int_0^t e^{-\gamma u} h(u) du \right] dt, \\ &= n \int_0^\infty e^{-nt} \left[\int_0^t e^{-\gamma u} h(u) du \right] dt, \end{aligned}$$

and thus it follows from (2.4) that

$$\int_0^\infty e^{-nt} \phi(t) dt = 0,$$

where

$$\phi(t) = \int_0^t e^{-\gamma t} h(t) dt. \quad (2.5)$$

In (2.5) put $x = e^{-t}$, $\psi(x) = \phi[\ln(1/x)]$. Then $\psi(x)$ is continuous in the closed interval $[0, 1]$, since we take

$$\psi(0) = \lim_{t \rightarrow \infty} \phi(t) \quad \text{and} \quad \psi(1) = \phi(0) = 0.$$

Also

$$\int_0^1 x^{n-1} \psi(x) dx = 0, \quad n = 1, 2, \dots$$

It follows from the lemma that $\psi(x) \equiv 0$ in $0 \leq x \leq 1$, and therefore

$$\phi(t) = \int_0^t e^{-\gamma t} h(t) dt = 0, \quad \text{when } t \geq 0. \quad (2.6)$$

Because $e^{-\gamma t} h(t)$ is continuous when $t \geq 0$, it follows from (2.6) that $e^{-\gamma t} h(t) = 0$ when $t \geq 0$, i.e. $h(t) = 0$, when $t \geq 0$. Consequently, $g(t) = f(t)$ when $t \geq 0$ and the theorem is proved. ■

The theorem gives us some confidence that a given Laplace transform $\bar{f}(s)$ will uniquely determine $f(t)$ if exact methods are used to determine $\mathcal{L}^{-1}\{\bar{f}(s)\}$. As Bellman and Roth [18] have pointed out Laplace transform inversion is, in many respects, an ill-conditioned problem. They give the examples of

$$\bar{f}_1(s) = \mathcal{L} \left\{ \frac{a}{2\sqrt{\pi}} \frac{e^{-a^2/4t}}{t^{3/2}} \right\} = e^{-a\sqrt{s}},$$

and

$$\bar{f}_2(s) = \mathcal{L}\{\sin bt\} = b/(s^2 + b^2).$$

The transform $\bar{f}_1(s)$ is uniformly bounded by 1 for all positive s and a whilst the function $f_1(t)$ has a maximum at $t = a^2/6$ and steadily decreases to zero. In fact, as $a \rightarrow 0$ it becomes more steadily spiked in the vicinity of $t = 0$ and provides a good approximation (after scaling) to the impulse function $\delta(t)$. The transform $\bar{f}_2(s)$ is uniformly bounded by $1/b$ for all positive s and b and is clearly the transform of a function which oscillates more and more rapidly as b increases but which is always bounded by 1. From the above analysis it follows that the function

$$1 + 10^{-20} f_1(t) + \sin 10^{20} t,$$

will have the same Laplace transform as $f(t) = 1$ to almost 20 significant digits when $a = 1$. The implication is that the spike behaviour, represented by the function $10^{-20} f_1(t)$, and the extremely rapid oscillations, represented by $\sin 10^{20} t$, are virtually impossible to be filtered out by numerical techniques. In what follows we shall assume, for the most part, that our given functions are essentially smooth.

2.2 The Bromwich Inversion Theorem

In the previous chapter we saw that we could determine the function $f(t)$ from its Laplace transform $\bar{f}(s)$ provided that it was possible to express $\bar{f}(s)$ in terms of simpler functions with known inverse transforms. This is essentially a haphazard process and we now give a direct method which has its basis in the following theorem :-

Theorem 2.2 The Inversion Theorem.

Let $f(t)$ have a continuous derivative and let $|f(t)| < Ke^{\gamma t}$ where K and γ are positive constants. Define

$$\bar{f}(s) = \int_0^\infty e^{-st} f(t) dt, \quad \Re s > \gamma. \quad (2.7)$$

Then

$$f(t) = \frac{1}{2\pi i} \lim_{T \rightarrow \infty} \int_{c-iT}^{c+iT} e^{st} \bar{f}(s) ds, \quad \text{where } c > \gamma \quad (2.8)$$

or

$$f(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \bar{f}(s) ds. \quad (2.8')$$

Proof. We have

$$\begin{aligned} I &= \frac{1}{2\pi i} \int_{c-iT}^{c+iT} e^{st} \bar{f}(s) ds = \frac{1}{2\pi i} \int_{c-iT}^{c+iT} e^{st} ds \int_0^\infty e^{-su} f(u) du, \\ &= \frac{1}{2\pi i} \int_0^\infty f(u) du \int_{c-iT}^{c+iT} e^{s(t-u)} ds, \end{aligned}$$

the change in order of integration being permitted since we have uniform convergence. Thus

$$\begin{aligned} I &= \frac{1}{2\pi i} \int_0^\infty \frac{f(u) du}{t-u} \left(e^{(\gamma+iT)(t-u)} - e^{(\gamma-iT)(t-u)} \right), \\ &= \frac{1}{\pi} \int_0^\infty e^{\gamma(t-u)} f(u) \frac{\sin T(t-u)}{t-u} du. \end{aligned}$$

Now let $u = t + \theta$, $\mathfrak{F}(\theta) = e^{-\gamma\theta} f(t + \theta)$. The right hand side of the integral then becomes

$$\frac{1}{\pi} \int_{-t}^\infty \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta. \quad (2.9)$$

We divide the integral in (2.9) into two parts \int_0^∞ and \int_{-t}^0 . We write

$$\begin{aligned} \int_0^\infty \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta &= \mathfrak{F}(0) \int_0^\delta \frac{\sin T\theta}{\theta} d\theta + \int_0^\delta \frac{\mathfrak{F}(\theta) - \mathfrak{F}(0)}{\theta} \sin T\theta d\theta \\ &\quad + \int_\delta^X \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta + \int_X^\infty \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta. \end{aligned} \quad (2.10)$$

We can choose δ small and X large so that

$$\left| \int_0^\delta \frac{\mathfrak{F}(\theta) - \mathfrak{F}(0)}{\theta} \sin T\theta d\theta \right| < \epsilon,$$

and

$$\left| \int_X^\infty \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta \right| < \epsilon,$$

for all T . Next consider

$$\int_\delta^X \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta.$$

Integrating by parts

$$\begin{aligned} \int_\delta^X \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta &= \left[-\frac{\cos T\theta}{T\theta} \mathfrak{F}(\theta) \right]_\delta^X + \frac{1}{T} \int_\delta^X \cos T\theta \frac{d}{d\theta} \left(\frac{\mathfrak{F}(\theta)}{\theta} \right) d\theta, \\ &= O(1/T), \end{aligned}$$

since each term involves $1/T$ and the integral is bounded. Again,

$$\begin{aligned} \int_0^\delta \frac{\sin T\theta}{\theta} d\theta &= \int_0^{T\delta} \frac{\sin \phi}{\phi} d\phi, \quad (\phi = T\theta) \\ &= \frac{\pi}{2} + O\left(\frac{1}{T}\right), \end{aligned}$$

since we know that

$$\int_0^\infty \frac{\sin \phi}{\phi} d\phi = \frac{\pi}{2}.$$

Combination of the above results gives

$$\lim_{T \rightarrow \infty} \int_0^\infty \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta = \frac{1}{2} \pi \mathfrak{F}(0) = \frac{1}{2} \pi f(t).$$

Similarly we can express

$$\begin{aligned} \int_{-t}^0 \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta &= \int_{-t}^{-\delta} \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta + \mathfrak{F}(0) \int_\delta^0 \frac{\sin T\theta}{\theta} d\theta \\ &\quad + \int_\delta^0 \frac{\mathfrak{F}(\theta) - \mathfrak{F}(0)}{\theta} \sin T\theta d\theta. \end{aligned}$$

A similar argument to that used previously yields

$$\lim_{T \rightarrow \infty} \int_{-t}^0 \mathfrak{F}(\theta) \frac{\sin T\theta}{\theta} d\theta = \frac{1}{2} \pi f(t).$$

The inversion formula follows by adding the two parts of the integral and dividing by π . ■

In particular, we note that if $f(t)$ is a real function we can write (2.8') in the alternative forms

$$f(t) = \frac{e^{ct}}{\pi} \int_0^\infty [\Re\{f(c+i\omega)\} \cos t\omega - \Im\{f(c+i\omega)\} \sin t\omega] d\omega, \quad (2.11)$$

$$= \frac{2e^{ct}}{\pi} \int_0^\infty \Re\{f(c+i\omega)\} \cos t\omega d\omega, \quad (2.12)$$

$$= \frac{-2e^{ct}}{\pi} \int_0^\infty \Im\{f(c+i\omega)\} \sin t\omega d\omega. \quad (2.13)$$

It has been assumed that the function $f(t)$ is continuous and differentiable. However, it may be shown that where $f(t)$ has a finite number of discontinuities and t is such a point then the inversion formula is

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \bar{f}(s) ds = \frac{1}{2} [f(t-) + f(t+)]. \quad (2.14)$$

An analogous result to (2.8) holds for the inversion of the two-dimensional Laplace transform, namely:-

Theorem 2.3 The Two-dimensional Inversion Formula.

Suppose $f(t_1, t_2)$ possesses first order partial derivatives $\partial f/\partial t_1$ and $\partial f/\partial t_2$ and second order derivative $\partial^2 f/\partial t_1 \partial t_2$ and there exist positive constants M, γ_1, γ_2 such that for all $0 < t_1, t_2 < \infty$

$$|f(t_1, t_2)| < M e^{\gamma_1 t_1 + \gamma_2 t_2}, \quad \left| \frac{\partial^2 f}{\partial t_1 \partial t_2} \right| < M e^{\gamma_1 t_1 + \gamma_2 t_2}.$$

Then if

$$\bar{f}(s_1, s_2) = \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} f(t_1, t_2) dt_1 dt_2,$$

we have

$$f(t_1, t_2) = \lim_{\substack{T_1 \rightarrow \infty \\ T_2 \rightarrow \infty}} \frac{1}{(2\pi i)^2} \int_{c_1 - iT_1}^{c_1 + iT_1} \int_{c_2 - iT_2}^{c_2 + iT_2} e^{s_1 t_1 + s_2 t_2} \bar{f}(s_1, s_2) ds_1 ds_2, \quad (2.15)$$

or

$$f(t_1, t_2) = \frac{1}{(2\pi i)^2} \int_{c_1 - i\infty}^{c_1 + i\infty} \int_{c_2 - i\infty}^{c_2 + i\infty} e^{s_1 t_1 + s_2 t_2} \bar{f}(s_1, s_2) ds_1 ds_2, \quad (2.16)$$

where $c_1 > \gamma_1$ and $c_2 > \gamma_2$. ■

A proof of this theorem can be found in Ditkin and Prudnikov [67].

Traditionally the inversion theorem has been applied by resorting to the calculus of residues. If a function $g(s)$ is regular inside a closed contour \mathcal{C} except

for a finite number of poles located at s_1, s_2, \dots, s_n then a well-known theorem of Cauchy informs us that

$$\int_{\mathcal{C}} g(s) ds = 2\pi i \sum_{k=1}^n R_k, \quad (2.17)$$

where

$$R_k = \text{residue of } g(s) \text{ at } s = s_k, \quad (2.18)$$

$$= \lim_{s \rightarrow s_k} (s - s_k) g(s), \quad (2.19)$$

if s_k is a simple pole. If s_k is a pole of order m then

$$R_k = \frac{1}{(m-1)!} \left[\frac{d^{m-1}}{ds^{m-1}} \{ (s - s_k)^m g(s) \} \right]_{s=s_k}. \quad (2.20)$$

Another useful application of Cauchy's theorem which follows from (2.17) is that if \mathcal{C}_1 and \mathcal{C}_2 are closed curves such that $\mathcal{C}_1 \subset \mathcal{C}_2$ then

$$\int_{\mathcal{C}_2} g(s) ds = \int_{\mathcal{C}_1} g(s) ds + 2\pi i \sum_{k=1}^n R_k, \quad (2.21)$$

where R_k denotes the residue at the pole $s = s_k$ which lies in the region $\mathcal{C}_2 - \mathcal{C}_1$. In particular, we can establish that if $\mathfrak{B} := \{s = c + it, -\infty < t < \infty\}$ and $\mathfrak{B}' := \{s = c' + it, -\infty < t < \infty\}$ where $c' < c$ then

$$\int_{\mathfrak{B}} g(s) ds = \int_{\mathfrak{B}'} g(s) ds + 2\pi i \sum_{k=1}^n R_k, \quad (2.22)$$

where R_k is the residue at the pole s_k which lies in the strip $c' < \Re s < c$.

In a large number of applications to determine the inverse transform we employ a contour \mathcal{C} which consists of a circular arc Γ of radius R cut off by the line $\Re s = \gamma$, as in Figure 2.1.

If $\bar{f}(s)$ satisfies the conditions of the following lemma then the lemma implies that $f(t)$ is determined by the sum of the residues at all singularities (i.e. poles) to the left of $\Re s = \gamma$.

Lemma 2.2 *If $|\bar{f}(s)| < CR^{-\nu}$ when $s = Re^{i\theta}$, $-\pi \leq \theta \leq \pi$, $R > R_0$, where R_0 , C and $\nu(> 0)$ are constants then, for $t > 0$,*

$$\int_{\Gamma_1} e^{st} \bar{f}(s) ds \rightarrow 0 \quad \text{and} \quad \int_{\Gamma_2} e^{st} \bar{f}(s) ds \rightarrow 0,$$

as $R \rightarrow \infty$ where Γ_1 and Γ_2 are respectively the arcs BCD and DEA of Γ .

Proof. Consider first

$$I_{\Gamma_1} = \int_{\Gamma_1} e^{st} \bar{f}(s) ds.$$

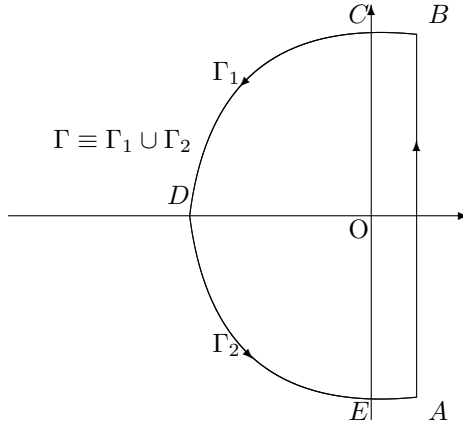


Figure 2.1: The standard Bromwich contour

The arc Γ_1 is made up of the arcs BC and CD . On BC , θ varies between $\alpha = \cos^{-1}(\gamma/R)$ and $\pi/2$. Thus

$$\begin{aligned} |I_{BC}| &< e^{\gamma t} \cdot \frac{C}{R^\nu} \cdot \int_{\alpha}^{\pi/2} d\theta, \\ &= \frac{C e^{\gamma t}}{R^\nu} R \sin^{-1}(\gamma/R), \\ &\rightarrow 0, \quad \text{as } R \rightarrow \infty, \end{aligned}$$

since, as $R \rightarrow \infty$, $R \sin^{-1}(\gamma/R) \rightarrow \gamma$.

For the arc CD ,

$$\begin{aligned} |I_{CD}| &< \frac{C}{R^\nu} \cdot R \int_{\pi/2}^{\pi} e^{Rt \cos \theta} d\theta, \\ &= \frac{C}{R^\nu} \cdot R \int_0^{\pi/2} e^{-Rt \sin \phi} d\phi, \end{aligned}$$

and, since $\sin \phi / \phi \geq 2/\pi$, $0 < \phi \leq \pi/2$,

$$\begin{aligned} &< \frac{C}{R^\nu} \cdot R \int_0^{\pi/2} e^{-2Rt\phi/\pi} d\phi, \\ &< \frac{\pi C}{2tR^\nu}. \end{aligned}$$

As $t > 0$ we see that $|I_{BC}| \rightarrow 0$ as $R \rightarrow \infty$. The same reasoning shows that the integrals over the arcs DE and EA can be made as small as we please and thus we have established the lemma. \blacksquare

We give some examples to illustrate the application of the inversion theorem.

Example 2.1 Find $\mathcal{L}^{-1}\{1/s(s-1)^3\}$.

This example was considered by other means in the previous chapter. It is clear from the form of $\bar{f}(s)$ that it has an isolated pole at $s = 0$ and a pole of order 3 at $s = 1$. If we take \mathcal{C} to be the contour in Figure 2.1 with $\gamma > 1$ then, with our previous notation for residues,

$$\int_{\mathcal{C}} e^{st} \bar{f}(s) ds = 2\pi i (R_1 + R_2),$$

where

$$R_1 = \lim_{s \rightarrow 0} \frac{(s-0)e^{st}}{s(s-1)^3},$$

and

$$R_2 = \lim_{s \rightarrow 1} \left[\frac{1}{2!} \frac{d^2}{ds^2} \left(\frac{(s-1)^3 e^{st}}{s(s-1)^3} \right) \right],$$

giving

$$R_1 = -1 \quad \text{and} \quad R_2 = e^t - te^t + \frac{1}{2}t^2 e^t.$$

Now let the radius of the circular section Γ of \mathcal{C} tend to infinity and we obtain

$$f(t) = R_1 + R_2 = -1 + e^t(1 - t + \frac{1}{2}t^2),$$

which is exactly the result obtained previously.

Now consider the following problem.

Example 2.2 Determine $\mathcal{L}^{-1}(1/s) \tanh \frac{1}{4}sT$.

This is not a rational function where we can apply the technique of partial fractions and we thus have to resort to the Inversion Theorem. Since $\tanh x = \sinh x / \cosh x$ we see that $e^{st} \bar{f}(s)$ has poles where $\cosh \frac{1}{4}sT = 0$, i.e., $s = s_n = 2i(2n+1)\pi/T$, $n = 0, \pm 1, \pm 2, \dots$. Note that $s = 0$ is not a pole because $\sinh \frac{1}{4}sT/s \rightarrow \frac{1}{4}T$ as $s \rightarrow 0$. The residue R_n at a typical pole s_n is given by

$$R_n = \lim_{s \rightarrow s_n} (s - s_n) \frac{e^{st} \sinh \frac{1}{4}sT}{s \cosh \frac{1}{4}sT}.$$

Application of l'Hôpital's rule gives

$$\begin{aligned} R_n &= \lim_{s \rightarrow s_n} \frac{e^{st} \sinh \frac{1}{4}sT}{\frac{1}{4}sT \sinh \frac{1}{4}sT}, \\ &= \frac{4e^{s_n t}}{s_n T} = 2e^{2(2n+1)i\pi t/T} / (2n+1)i\pi. \end{aligned}$$

Treating the contour \mathcal{C} as before we find

$$f(t) = \sum_{-\infty}^{\infty} R_n,$$

which simplifies to

$$f(t) = \frac{4}{\pi} \sum_0^{\infty} \frac{\sin(4n+2)\pi t/T}{2n+1}.$$

This turns out to be the Fourier series representation of the square wave function so that we have no contradiction with the results of the last chapter.

Another example where the Inversion Theorem is required is in modelling the vibration of a beam.

Example 2.3 A beam of length L has one end ($x = 0$) fixed and is initially at rest. A constant force F_0 per unit area is applied longitudinally at the free end. Find the longitudinal displacement of any point x of the beam at any time $t > 0$.

Denote by $y(x, t)$ the longitudinal displacement of any point x of the beam at time t . Then it can be shown that $y(x, t)$ satisfies the partial differential equation

$$\frac{\partial^2 y}{\partial t^2} = c^2 \frac{\partial^2 y}{\partial x^2}, \quad 0 < x < L, \quad t > 0,$$

where c is a constant, subject to the boundary conditions

$$\begin{aligned} y(x, 0) &= 0, & \frac{\partial}{\partial t} y(x, 0) &= 0, \\ y(0, t) &= 0, & \frac{\partial}{\partial x} y(L, t) &= F_0/E, \end{aligned}$$

E being Young's modulus for the beam.

Taking Laplace transforms of the differential equation we have

$$s^2 \bar{y}(x, s) - sy(x, 0) - \frac{\partial}{\partial t} y(x, 0) = c^2 \frac{d^2 \bar{y}}{dx^2},$$

or

$$\frac{d^2 \bar{y}}{dx^2} - \frac{s^2}{c^2} \bar{y} = 0,$$

together with

$$\bar{y}(0, s) = 0, \quad \frac{d}{dx} \bar{y}(L, s) = \frac{F_0}{Es}.$$

The general solution of the ordinary differential equation is

$$\bar{y}(x, s) = A \cosh(sx/c) + B \sinh(sx/c).$$

The boundary condition $\bar{y}(0, s) = 0$ implies $A = 0$ and the remaining condition yields

$$B = cF_0/Es^2 \cosh(sL/c),$$

so that

$$\bar{y}(x, s) = \frac{cF_0}{E} \cdot \frac{\sinh(sx/c)}{s^2 \cosh(sL/c)}.$$

Now consider

$$\int_{\mathcal{C}} e^{st} \bar{y}(x, s) ds,$$

where \mathcal{C} does not pass through any poles of the integrand. The integrand appears to have a double pole at $s = 0$ but as $(\sinh s/s) \rightarrow 1$ as $s \rightarrow 0$ it is clear that the pole is in fact simple. There are also simple poles where

$$\cosh(sL/c) = 0,$$

i.e.

$$s = s_n = (n - \frac{1}{2})\pi ic/L, \quad n = 0, \pm 1, \pm 2, \dots$$

By choosing R the radius of the circular part of \mathcal{C} to be $n\pi c/L$ we ensure that there are no poles on the boundary of \mathcal{C} . We also have to check that the integrand satisfies the conditions of the Lemma. Carslaw and Jaeger [31] establish this for similar problems and the reader is referred to that text to obtain an outline of the proof. The residue at $s = 0$ is

$$\lim_{s \rightarrow 0} (s - 0) \frac{cF_0}{E} \cdot \frac{e^{st} \sinh(sx/c)}{s^2 \cosh(sL/c)} = \lim_{s \rightarrow 0} \frac{cF_0}{E} \frac{e^{st} (x/c) \cosh(sx/c)}{\cosh(sL/c)} = \frac{F_0 x}{E}.$$

The residue, R_n , at $s = s_n$ is given by

$$\begin{aligned} R_n &= \lim_{s \rightarrow s_n} (s - s_n) \frac{cF_0}{E} \left[\frac{e^{st} \sinh(sx/c)}{s^2 \cosh(sL/c)} \right], \\ &= \lim_{s \rightarrow s_n} \frac{cF_0}{E} \cdot \frac{e^{st} \sinh(sx/c)}{s^2 (L/c) \sinh(sL/c)}, \\ &= \frac{c^2 F_0}{EL} \cdot \frac{e^{(n-\frac{1}{2})\pi ict/L} \sin(n - \frac{1}{2})\pi x/L}{-(n - \frac{1}{2})^2 (\pi c/L)^2 \sin(n - \frac{1}{2})\pi}, \end{aligned}$$

after simplification. Note the use of l'Hôpital's rule in the determination of the above residues.

Now let $R \rightarrow \infty$ then, because the integral over the curved part of \mathcal{C} tends to zero by the Lemma, it follows that

$$y(x, t) = \frac{F_0 x}{E} + \sum_{-\infty}^{\infty} \frac{(-1)^n 4F_0 L}{E\pi^2} \cdot \frac{e^{(n-\frac{1}{2})\pi ict/L} \sin(n - \frac{1}{2})\pi x/L}{(2n - 1)^2}.$$

In the summation consider addition of the terms $n = m$ and $n = -m + 1$ ($m = 1, 2, \dots$). We find that

$$y(x, t) = \frac{F_0}{E} \left[x + \frac{8L}{\pi^2} \sum_{m=1}^{\infty} \frac{(-1)^n}{(2n - 1)^2} \sin \frac{(2n - 1)\pi x}{2L} \cos \frac{(2n - 1)\pi ct}{2L} \right].$$

While we obviously have a great deal of satisfaction in achieving a result like this we have to bear in mind that it is no easy task to sum the series obtained.

We now consider another example which requires a modification of the Bromwich contour.

Example 2.4 Consider the solution of the partial differential equation

$$\frac{\partial y}{\partial t} = \frac{\partial^2 y}{\partial x^2}, \quad x > 0, \quad t > 0,$$

with

$$\begin{aligned} y &= 1, & \text{when } x = 0, \quad t > 0, \\ y &= 0, & \text{when } x > 0, \quad t = 0. \end{aligned}$$

This type of equation arises when considering the flow of heat in a semi-infinite solid. Taking the Laplace transform of the partial differential equation we obtain

$$\frac{d^2 \bar{y}}{dx^2} - s\bar{y} = 0, \quad x > 0,$$

with initial condition

$$\bar{y} = 1/s, \quad \text{when } x = 0.$$

The solution of this ordinary differential equation which is finite as $x \rightarrow \infty$ is

$$\bar{y} = \frac{1}{s} \exp(-x\sqrt{s}),$$

and the inversion theorem gives

$$y = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{st-x\sqrt{s}} \frac{ds}{s}. \quad (2.23)$$

The integrand in (2.23) has a branch point at the origin and it is thus necessary to choose a contour which does not enclose the origin. We deform the Bromwich contour so that the circular arc Γ_1 is terminated just short of the horizontal axis and the arc Γ_2 starts just below the horizontal axis. In between the contour follows a path DF which is parallel to the axis, followed by a circular arc Γ' enclosing the origin and a return section $F'D'$ parallel to the axis meeting the arc Γ_2 — see Figure 2.2.

As there are no poles inside this contour \mathcal{C} we have

$$\int_{\mathcal{C}} e^{st-x\sqrt{s}} \frac{ds}{s} = 0.$$

Now on Γ_1 and Γ_2

$$\left| \frac{1}{s} e^{-x\sqrt{s}} \right| < 1/|s|,$$

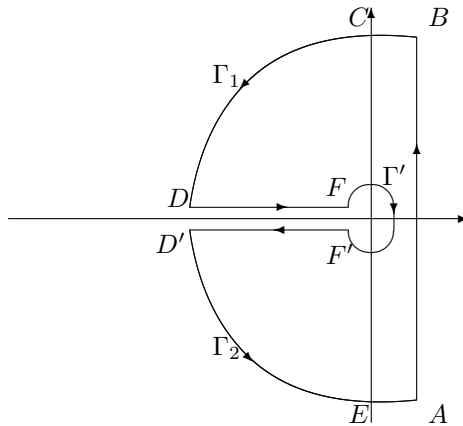


Figure 2.2: A modified Bromwich contour

so that the integrals over these arcs tend to zero as $R \rightarrow \infty$. Over the circular arc Γ' as its radius $r \rightarrow 0$, we have

$$\begin{aligned} \int_{\Gamma'} e^{st-x\sqrt{s}} \frac{ds}{s} &\rightarrow \int_{\pi}^{-\pi} e^{re^{i\theta}-x\sqrt{re^{i\theta/2}}} \frac{ire^{i\theta} d\theta}{re^{i\theta}}, \quad (r \rightarrow 0), \\ &\rightarrow \int_{\pi}^{-\pi} i d\theta = -2\pi i. \end{aligned}$$

Over the horizontal sections DF and $F'D'$ the integrals are

$$\int_R^r e^{ue^{i\pi}t-x\sqrt{ue^{i\pi/2}}} \frac{du}{u} \quad \text{and} \quad \int_r^R e^{ue^{-i\pi}t-x\sqrt{ue^{-i\pi/2}}} \frac{du}{u}.$$

As $r \rightarrow 0$ and $R \rightarrow \infty$ their sum becomes

$$\int_0^\infty e^{-ut} [-e^{-ix\sqrt{u}} + e^{ix\sqrt{u}}] \frac{du}{u},$$

i.e.,

$$2i \int_0^\infty e^{-ut} \sin x\sqrt{u} \frac{du}{u},$$

or

$$4i \int_0^\infty e^{-v^2t} \sin vx \frac{dv}{v}.$$

Now from Gradshteyn and Ryzhik [102] we know that

$$\int_0^\infty e^{-v^2t} \sin vx \frac{dv}{v} = \sqrt{\pi} \int_0^{x/2\sqrt{t}} e^{-v^2} dv.$$

Hence

$$y = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{st-x\sqrt{s}} \frac{ds}{s} = 1 - \frac{2}{\sqrt{\pi}} \int_0^{x/2\sqrt{t}} e^{-v^2} dv,$$

yielding

$$y = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{t}}\right).$$

An alternative method to contour integration for finding inverse transforms has been given by Goldenberg [100]. This depends on $\bar{f}(s)$ satisfying a differential equation of the form

$$\alpha_n(s) \frac{d^n \bar{f}}{ds^n} + \alpha_{n-1}(s) \frac{d^{n-1} \bar{f}}{ds^{n-1}} + \cdots + \alpha_1(s) \frac{d\bar{f}}{ds} + \alpha_0(s) \bar{f} = \beta(s),$$

where the $\alpha_i(s)$ ($i = 0, 1, \dots, n$) are polynomials of degree at most i in s and the inverse transform of $\beta(s)$ is known.

Example 2.5 Determine $f(t)$ when

$$\bar{f}(s) = \frac{1}{s} \tan^{-1}(s+a), \quad a > 0.$$

Writing the above as

$$s\bar{f}(s) = \tan^{-1}(s+a),$$

differentiation produces

$$s \frac{d\bar{f}}{ds} + \bar{f} = \frac{1}{(s+a)^2 + 1}.$$

Inversion yields

$$-t \frac{df}{dt} = e^{-at} \sin t,$$

and hence

$$f(t) = f(0) - \int_0^t \frac{e^{-at} \sin t}{t} dt.$$

As $\bar{f}(s)$ satisfies the conditions of Theorem 2.5 we have

$$f(0) = \lim_{s \rightarrow \infty} s\bar{f}(s) = \lim_{s \rightarrow \infty} \tan^{-1}(s+a) = \pi/2.$$

Thus

$$f(t) = \frac{\pi}{2} - \int_0^t \frac{e^{-at} \sin t}{t} dt.$$

Goldenberg shows that this result can be expressed in terms of the complex exponential integral $E_1(z)$ and finds

$$\mathcal{L}^{-1} \left\{ \frac{1}{s} \tan^{-1}(s+a) \right\} = \tan^{-1} a - \Im E_1(at + it).$$

2.3 The Post-Widder Inversion Formula

The Bromwich inversion formula of the last section is not the only way to represent the inverse transform as we also have the following result of Post [190] and Widder [253]:-

Theorem 2.4 The Post-Widder Theorem.

If the integral

$$\bar{f}(s) = \int_0^\infty e^{-su} f(u) du, \quad (2.24)$$

converges for every $s > \gamma$, then

$$f(t) = \lim_{n \rightarrow \infty} \frac{(-1)^n}{n!} \left(\frac{n}{t}\right)^{n+1} \bar{f}^{(n)}\left(\frac{n}{t}\right), \quad (2.25)$$

for every point $t(> 0)$ of continuity of $f(t)$.

The advantage of formula (2.25) lies in the fact that f is expressed in terms of the value of \bar{f} and its derivatives on the real axis. A big disadvantage however is that convergence to $f(t)$ is very slow. We shall assume that the integral (2.24) converges absolutely but this restriction is only imposed in order to simplify the proof.

Proof. Differentiating (2.24) with respect to s we obtain, after substituting $s = n/t$,

$$\bar{f}^{(n)}\left(\frac{n}{t}\right) = (-1)^n \int_0^\infty u^n \exp\left(-\frac{nu}{t}\right) f(u) du.$$

The right hand side of (2.25) is thus

$$\lim_{n \rightarrow \infty} \frac{n^{n+1}}{e^n n!} \frac{1}{t} \int_0^\infty \left[\frac{u}{t} \exp\left(1 - \frac{u}{t}\right)\right]^n f(u) du.$$

By Stirling's approximation for $n!$ we know that

$$\lim_{n \rightarrow \infty} \frac{n^n \sqrt{2\pi n}}{e^n n!} = 1,$$

and thus we have to prove that

$$f(t) = \lim_{n \rightarrow \infty} \frac{1}{\sqrt{2\pi} t} \int_0^\infty n^{1/2} \left[\frac{u}{t} \exp\left(1 - \frac{u}{t}\right)\right]^n f(u) du. \quad (2.26)$$

Let δ be a fixed positive number such that $\delta < t$ and expand the integral in (2.26) in the form

$$\int_0^\infty = \int_0^{t-\delta} + \int_{t-\delta}^{t+\delta} + \int_{t+\delta}^\infty = I_1 + I_2 + I_3.$$

As the function

$$x \exp(1 - x), \quad (2.27)$$

increases monotonically from 0 to 1 in $[0, 1]$ we have

$$\frac{t-\delta}{t} \exp\left(1 - \frac{t-\delta}{t}\right) = \eta < 1,$$

and hence

$$|I_1| \leq n^{1/2} \eta^n \int_0^{t-\delta} |f(u)| du,$$

which implies that $I_1 \rightarrow 0$ as $n \rightarrow \infty$. Again, in $[1, \infty)$, the function (2.27) decreases monotonically from 1 to 0 and thus

$$\frac{t+\delta}{t} \exp\left(1 - \frac{t+\delta}{t}\right) = \zeta < 1,$$

which implies that

$$I_3 = n^{1/2} \int_{t+\delta}^{\infty} \left[\frac{u}{t} \exp\left(1 - \frac{u}{t}\right)\right]^{n-n_0} \left[\frac{u}{t} \exp\left(1 - \frac{u}{t}\right)\right]^{n_0} f(u) du,$$

so that

$$\begin{aligned} |I_3| &\leq n^{1/2} \zeta^{n-n_0} \int_{t+\delta}^{\infty} \left[\frac{u}{t} \exp\left(1 - \frac{u}{t}\right)\right]^{n_0} |f(u)| du, \\ &\leq n^{1/2} \zeta^n (e/\zeta)^{n_0} \int_{t+\delta}^{\infty} \left(\frac{u}{t}\right)^{n_0} \exp\left(-\frac{n_0 u}{t}\right) |f(u)| du. \end{aligned}$$

This last integral is convergent if $n_0/t > \gamma$. Hence $I_3 \rightarrow 0$ as $n \rightarrow \infty$. We have still to consider I_2 . Let t be a point of continuity of f . Then, given any $\varepsilon > 0$ we can choose $\delta > 0$ such that

$$f(t) - \varepsilon < f(u) < f(t) + \varepsilon \quad \text{for} \quad t - \delta < u < t + \delta.$$

Then

$$(f(t) - \varepsilon)I < I_2 < (f(t) + \varepsilon)I, \quad (2.28)$$

where

$$I = \int_{t-\delta}^{t+\delta} n^{1/2} \left[\frac{u}{t} \exp\left(1 - \frac{u}{t}\right)\right]^n du.$$

In the preceding argument we have not specified the function $f(t)$ and the results hold generally. In particular, when $f(t) = 1$, $\bar{f}(s) = 1/s$, $\bar{f}^{(n)}(s) = (-1)^n n! / s^{n+1}$ giving

$$\bar{f}^{(n)}(n/t) = (-1)^n n! (t/n)^{n+1}.$$

Substituting in (2.25) we find that (2.25) holds. Since (2.25) and (2.26) are equivalent then (2.26) must also hold for $f(t) = 1$. Thus

$$1 = \lim_{n \rightarrow \infty} \frac{1}{\sqrt{2\pi t}} (I_1 + I_2 + I_3) \quad \text{for} \quad f(t) = 1.$$

Now we have already proved that I_1 and I_3 tend to 0 whatever the value of $f(t)$ and, when $f(t) = 1$, $I_2 = I$. Consequently we get

$$1 = \lim_{n \rightarrow \infty} \frac{1}{\sqrt{2\pi t}} I. \quad (2.29)$$

By (2.28) we find that the lower and upper limits of the integral in (2.26) lie between $f(t) - \varepsilon$ and $f(t) + \varepsilon$. This implies that both limits equal $f(t)$ as ε is arbitrarily small. Hence (2.26) and the equivalent formula (2.25) are proved. ■

Example 2.6 Given $\bar{f}(s) = 1/(s+1)$. Determine $f(t)$.

We find by repeated differentiation that

$$\bar{f}^{(n)}(s) = (-1)^n \frac{n!}{(s+1)^{n+1}}.$$

Thus

$$\begin{aligned} f(t) &= \lim_{n \rightarrow \infty} \frac{(-1)^n}{n!} \left(\frac{n}{t}\right)^{n+1} \frac{(-1)^n n!}{\left(\frac{n}{t} + 1\right)^{n+1}}, \\ &= \lim_{n \rightarrow \infty} \left(1 + \frac{t}{n}\right)^{-(n+1)}, \\ &= \lim_{n \rightarrow \infty} \left(1 + \frac{t}{n}\right)^{-n} \cdot \lim_{n \rightarrow \infty} \left(1 + \frac{t}{n}\right)^{-1} = e^{-t}. \end{aligned}$$

Jagerman [116] has established that the successive convergents

$$f_k(t) = s \frac{(-s)^{k-1} \bar{f}^{(k-1)}(s)}{(k-1)!} \Big|_{s=k/t}, \quad t > 0, \quad (2.30)$$

can be generated via the formula

$$s \bar{f}[s(1-z)] = \sum_{n \geq 1} f_n \left(\frac{n}{s}\right) z^{n-1}, \quad (2.31)$$

and this relationship will be the basis of alternative numerical methods for obtaining the inverse Laplace transform.

2.4 Initial and Final Value Theorems

Sometimes we know a Laplace transform $\bar{f}(s)$ and we are mainly interested in finding some properties of $f(t)$, in particular its limits as $t \rightarrow 0$ and $t \rightarrow \infty$ without the trouble of determining the complete theoretical solution. These are quite important properties to know and will be used in the development of some of the numerical methods which are discussed in later chapters.

Theorem 2.5 *The Initial Value theorem.*

If as $s \rightarrow \infty$, $\bar{f}(s) \rightarrow 0$, and, in addition,

$$f(t) \rightarrow f(0) \quad \text{as } t \rightarrow 0$$

and

$$e^{-st}f(t) \rightarrow 0 \quad \text{as } t \rightarrow \infty,$$

then

$$\lim_{s \rightarrow \infty} s\bar{f}(s) = \lim_{t \rightarrow 0} f(t). \quad (2.32)$$

Proof. We know that $\bar{f}(s)$ is defined by

$$\bar{f}(s) = \int_0^{\infty} e^{-st} f(t) dt, \quad (2.33)$$

and we assume that the integral is absolutely convergent if $s \geq \gamma$. Write (2.33) in the form

$$\bar{f}(s) = \int_0^{T_1} e^{-st} f(t) dt + \int_{T_1}^{T_2} e^{-st} f(t) dt + \int_{T_2}^{\infty} e^{-st} f(t) dt. \quad (2.34)$$

Then, given an arbitrarily small positive number ε , we can choose T_1 so small that

$$\left| \int_0^{T_1} e^{-st} f(t) dt \right| < \int_0^{T_1} e^{-st} |f(t)| dt < \frac{1}{3}\varepsilon, \quad s \geq \gamma$$

because of the absolute convergence of (2.33). For the same reason we can take T_2 so large that

$$\left| \int_{T_2}^{\infty} e^{-st} f(t) dt \right| < \int_{T_2}^{\infty} e^{-st} |f(t)| dt < \frac{1}{3}\varepsilon, \quad s \geq \gamma$$

Finally, we can choose s so large that

$$\left| \int_{T_1}^{T_2} e^{-st} f(t) dt \right| < e^{-sT_1} \int_{T_1}^{T_2} |f(t)| dt < \frac{1}{3}\varepsilon, \quad s \geq \gamma$$

It follows from (2.34) that

$$\lim_{s \rightarrow \infty} \bar{f}(s) = 0. \quad (2.35)$$

The theorem now follows on applying the above result to df/dt since, by (1.14), $\mathcal{L}\{df/dt\} = s\bar{f}(s) - f(0+)$. ■

Theorem 2.6 *The Final Value theorem.*

If $f(\gamma)$ exists, and $s \rightarrow \gamma+$ through real values, then

$$\bar{f}(s) \rightarrow \bar{f}(\gamma). \quad (2.36)$$

Further,

$$\lim_{s \rightarrow 0} \bar{f}(s) = \int_0^{\infty} f(t) dt, \quad (2.37)$$

$$\lim_{s \rightarrow 0} s \bar{f}(s) = \lim_{t \rightarrow \infty} f(t), \quad (2.38)$$

provided that the quantities on the right-hand sides of (2.37) and (2.38) exist and in addition, for (2.38), we require $e^{-st}f(t) \rightarrow 0$ as $t \rightarrow \infty$ and $f(t) \rightarrow f(0)$ as $t \rightarrow 0$.

Proof. We write

$$\begin{aligned} \left| \int_0^{\infty} e^{-\gamma t} f(t) dt - \int_0^{\infty} e^{-st} f(t) dt \right| &\leq \left| \int_0^T e^{-\gamma t} f(t) dt - \int_0^T e^{-st} f(t) dt \right| \\ &\quad + \left| \int_T^{\infty} e^{-\gamma t} f(t) dt \right| + \left| \int_T^{\infty} e^{-st} f(t) dt \right|. \end{aligned} \quad (2.39)$$

Given any arbitrarily small number ϵ the last two terms in (2.39) can be made less than $\epsilon/3$ by appropriate choice of T , by virtue of the fact that the infinite integrals on the left hand side are known to be convergent. Also, by continuity, we can find a positive number δ such that the first term on the right hand side of (2.39) is less than $\epsilon/3$ when $0 \leq s - \gamma \leq \delta$. It follows that

$$|\bar{f}(s) - \bar{f}(\gamma)| \leq \epsilon,$$

which proves (2.36). Condition (2.37) is just the case where $\gamma = 0$. Application of (2.37) to the function df/dt gives the result (2.38). Hence the theorem is proved. ■

Note that the theorem requires the right hand sides of (2.37) and (2.38) to exist for the left hand side to exist and be equal to it. The converse is not true as can be seen by the example $f(t) = \sin \omega t$. For this function

$$s \bar{f}(s) = \frac{\omega s}{s^2 + \omega^2}, \quad \lim_{s \rightarrow 0} s \bar{f}(s) = 0.$$

However, because of the oscillatory nature of $f(t)$

$$\lim_{t \rightarrow \infty} f(t) \quad \text{does not exist.}$$

If stronger conditions are imposed on $\bar{f}(s)$ (or $f(t)$) then the converse may be true.

Example 2.7 $\bar{f}(s) = 1/s(s + a)$, $a > 0$.

We can easily establish that

$$f(t) = (1/a)[1 - e^{-at}].$$

Thus

$$\lim_{t \rightarrow \infty} f(t) = 1/a.$$

Application of the theorem gives

$$\lim_{s \rightarrow 0} s\bar{f}(s) = \lim_{s \rightarrow 0} 1/(s + a) = 1/a,$$

which confirms the result obtained previously. Also, applying the initial value theorem gives

$$\lim_{s \rightarrow \infty} s\bar{f}(s) = \lim_{s \rightarrow \infty} 1/(s + a) = 0 = f(0),$$

which confirms the result that

$$\lim_{t \rightarrow 0} f(t) = 0.$$

2.5 Series and Asymptotic Expansions

In the previous section we were interested in estimating the limiting value of $f(t)$, if it existed, as $t \rightarrow 0$ and $t \rightarrow \infty$. In this section we give some results which are required for the development of certain numerical methods. In particular, we have

Theorem 2.7 *If $\bar{f}(s)$ can be expanded as an absolutely convergent series of the form*

$$\bar{f}(s) = \sum_{n=0}^{\infty} \frac{a_n}{s^{\lambda_n}}, \quad |s| > R \quad (2.40)$$

where the λ_n form an increasing sequence of numbers $0 < \lambda_0 < \lambda_1 < \dots \rightarrow \infty$ then

$$f(t) = \sum_{n=0}^{\infty} \frac{a_n t^{\lambda_n - 1}}{\Gamma(\lambda_n)}. \quad (2.41)$$

The series (2.41) converges for all real and complex t . ■

Another important result is:-

Theorem 2.8 *If $\bar{f}(s)$ can be expanded in the neighbourhood of $s = \alpha_i$, in the complex s -plane, in an absolutely convergent power series with arbitrary exponents*

$$\bar{f}(s) = \sum_{n=0}^{\infty} b_n (s - \alpha_i)^{\mu_n}, \quad -N < \mu_0 < \mu_1 < \dots \rightarrow \infty \quad (2.42)$$

then there exists a contribution to the asymptotic expansion of $f(t)$ as $t \rightarrow \infty$ of the form

$$e^{\alpha_i t} \sum_{n=0}^{\infty} \frac{b_n t^{-\mu_n - 1}}{\Gamma(-\mu_n)}, \quad (2.43)$$

where $1/\Gamma(-\mu_n) = 0$ if μ_n is a positive integer or zero. ■

See Doetsch [70] for proofs.

We end this section with a statement of Watson's lemma — see Olver [163] for a proof of this result.

Lemma 2.3 *Watson's Lemma*

Suppose that the function $f(t)$ satisfies

$$f(t) \sim \sum_{k=0}^{\infty} a_k t^{\alpha_k} \quad \text{as } t \rightarrow 0+,$$

where $-1 < \Re \alpha_0 < \Re \alpha_1 < \dots$, and $\lim_{k \rightarrow \infty} \Re \alpha_k = \infty$. Then, for any $\delta > 0$,

$$\bar{f}(s) \sim \sum_{k=0}^{\infty} \frac{a_k \Gamma(\alpha_k + 1)}{s^{\alpha_k + 1}} \quad \text{as } s \rightarrow \infty, \quad |\arg s| < \frac{1}{2}\pi - \delta.$$

■

2.6 Parseval's Formulae

It is well-known that if a function $f(x)$ possesses a Fourier series expansion, i.e.

$$f(x) = \frac{1}{2}a_0 + a_1 \cos x + b_1 \sin x + \dots + a_n \cos nx + b_n \sin nx + \dots, \quad -\pi < x < \pi$$

then

$$\frac{1}{\pi} \int_{-\pi}^{\pi} |f(x)|^2 dx = \frac{1}{2}a_0^2 + \sum_{i=1}^{\infty} (a_i^2 + b_i^2). \quad (2.44)$$

The result (2.44) is called Parseval's formula. A similar result holds for Fourier transforms, namely

$$\int_{-\infty}^{\infty} |\mathfrak{F}(\omega)|^2 d\omega = \int_{-\infty}^{\infty} |f(t)|^2 dt, \quad (2.45)$$

where $\mathfrak{F}(\omega)$ is the Fourier transform of $f(t)$ defined by

$$\mathfrak{F}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt, \quad -\infty < t < \infty$$

We also mention the associated Fourier sine and cosine transforms defined by

$$\begin{aligned} \mathfrak{F}_S(\omega) &= \sqrt{\frac{2}{\pi}} \int_0^{\infty} f(t) \sin \omega t dt, \\ \mathfrak{F}_C(\omega) &= \sqrt{\frac{2}{\pi}} \int_0^{\infty} f(t) \cos \omega t dt, \end{aligned}$$

We also recall at this point the inversion formulae for these transforms, namely

$$\begin{aligned} f(t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathfrak{F}(\omega) e^{-it\omega} d\omega, \\ f(t) &= \sqrt{\frac{2}{\pi}} \int_0^{\infty} \mathfrak{F}_S(\omega) \sin t\omega d\omega, \end{aligned}$$

and

$$f(t) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \mathfrak{F}_C(\omega) \cos t\omega d\omega.$$

We now establish formally the equivalent Parseval result for Laplace transforms

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} |\bar{f}(c+it)|^2 dt = \int_0^{\infty} e^{-2cu} [f(u)]^2 du. \quad (2.46)$$

We have

$$\begin{aligned} \int_{-\infty}^{\infty} |\bar{f}(c+it)|^2 dt &= \int_{-\infty}^{\infty} \bar{f}(c+it) \bar{f}(c-it) dt, \\ &= \int_{-\infty}^{\infty} \bar{f}(c+it) \left(\int_0^{\infty} f(u) e^{-(c-it)u} du \right) dt, \\ &= \int_0^{\infty} f(u) \left(\int_{-\infty}^{\infty} \bar{f}(c+it) e^{(c+it)u} dt \right) e^{-2cu} du, \\ &= \int_0^{\infty} f(u) \cdot 2\pi f(u) \cdot e^{-2cu} du, \\ &= 2\pi \int_0^{\infty} e^{-2cu} [f(u)]^2 du, \end{aligned}$$

which is equivalent to (2.46). This argument needs some justification and a more rigorous proof is given in Watson [246]. A useful source of information for proofs and additional theoretical results on Integral Transforms is Davies [59].

Chapter 3

The Method of Series Expansion

3.1 Expansion as a Power Series

We have already seen that if n is an integer

$$\mathcal{L}\{t^n\} = \frac{n!}{s^{n+1}}$$

and thus

$$\frac{t^n}{n!} = \mathcal{L}^{-1} \left\{ \frac{1}{s^{n+1}} \right\}, \quad n \geq 0.$$

Consequently, if we can express $\bar{f}(s)$ in the form

$$\bar{f}(s) = \frac{a_1}{s} + \frac{a_2}{s^2} + \cdots + \frac{a_n}{s^n} + \cdots \quad (3.1)$$

we have

$$f(t) = a_1 + a_2 t + a_3 \frac{t^2}{2!} + \cdots + a_n \frac{t^{n-1}}{(n-1)!} + \cdots \quad (3.2)$$

(see Theorem 2.7) and by computing this series we can, in theory, evaluate $f(t)$ for any t . We shall illustrate the method by examples.

Example 3.1 Given $\bar{f}(s) = 1/(1+s)$. Determine $f(t)$.
We write

$$\begin{aligned} \bar{f}(s) &= \frac{1}{s(1 + \frac{1}{s})} \\ &= \frac{1}{s} \left(1 - \frac{1}{s} + \frac{1}{s^2} - \frac{1}{s^3} + \cdots \right) \\ &= \frac{1}{s} - \frac{1}{s^2} + \frac{1}{s^3} - \frac{1}{s^4} + \cdots \end{aligned}$$

k	t	$S_1^{(k)}$
15	20	$2.0611536224827 \times 10^{-9}$
16	20	$2.0611536224387 \times 10^{-9}$

Table 3.1: Iterated Aitken algorithm $t = 20$, $f(s) = 1/(s + 1)$.

It follows that

$$f(t) = 1 - t + \frac{t^2}{2!} - \cdots + \frac{(-t)^n}{n!} + \cdots \quad (3.3)$$

The series for $f(t)$ converges for all t . However, for large t , there will be severe cancellation in the computation of the series. Thus when $t = 20$, for example, the largest term in the series is $O(10^7)$ whereas the value of $f(t)$ is $O(10^{-9})$ which indicates that 16 significant digits will be lost in the computation. Thus for this approach to be successful for large t we will require the use of multi-length arithmetic. Moreover, with 32 decimal digit arithmetic we would need to compute about 90 terms of the series in order to determine $f(t)$ correct to approximately 12 significant digits. However, we can bring into play Extrapolation Techniques (see Appendix §11.4) to speed up convergence. The iterated Aitken algorithm yields Table 3.1 . Since the exact solution is $f(t) = e^{-t}$ and $f(20) = 2.06115362243855 \cdots \times 10^{-9}$ the above table indicates that we have been able to achieve 20 decimal place accuracy with a knowledge of only 33 terms of the series (3.3). It would be virtually impossible, using a Fortran program and a computer with a word-length of 32 decimal digits, to evaluate $f(t)$ for $t = 50$ by direct computation of the series (3.3) as over 40 significant digits are lost in the computation. The extrapolation procedure is also quite likely to break down. If extended precision arithmetic is available, as for example with Maple or Mathematica, then it is possible to get very accurate results by computing (3.3).

We now give some other examples of the above technique.

Example 3.2 $\bar{f}(s) = 1/(s^2 + 1)$. Determine $f(t)$.

We now have

$$\begin{aligned} \bar{f}(s) &= \frac{1}{s^2(1 + (1/s^2))}, \\ &= \frac{1}{s^2} \left(1 - \frac{1}{s^2} + \frac{1}{s^4} - \frac{1}{s^6} + \cdots \right), \\ &= \frac{1}{s^2} - \frac{1}{s^4} + \frac{1}{s^6} - \frac{1}{s^8} + \cdots, \end{aligned}$$

and it follows that

$$f(t) = t - \frac{t^3}{3!} + \frac{t^5}{5!} - \frac{t^7}{7!} + \cdots \quad (= \sin t). \quad (3.4)$$

(3.4) is a series which converges for all t and here again direct evaluation of the series would present computational difficulties for large t but not to quite the same extent as in Example 3.1 as, for the most part, $f(t) = O(1)$.

Example 3.3 $\bar{f}(s) = e^{-a/s}/\sqrt{s}$. Determine $f(t)$.
Expansion of the term $e^{-a/s}$ yields

$$\begin{aligned}\bar{f}(s) &= \frac{1}{\sqrt{s}} \left(1 - \frac{a}{s} + \frac{a^2}{2!s^2} - \frac{a^3}{3!s^3} + \cdots \right), \\ &= \frac{1}{s^{1/2}} - \frac{a}{s^{3/2}} + \frac{a^2}{2!s^{5/2}} - \frac{a^3}{3!s^{7/2}} + \cdots.\end{aligned}$$

Now

$$\mathcal{L}^{-1} \left\{ \frac{1}{\sqrt{s}} \right\} = \frac{1}{\sqrt{\pi t}},$$

and

$$\mathcal{L}^{-1} \left\{ s^{-(n+\frac{1}{2})} \right\} = \frac{4^n n! t^{n-\frac{1}{2}}}{(2n)! \sqrt{\pi}},$$

so that

$$f(t) = \frac{1}{\sqrt{\pi t}} \left(1 - 2at + \frac{2}{3}a^2t^2 + \cdots + \frac{(-4at)^n}{(2n)!} + \cdots \right). \quad (3.5)$$

As $t \rightarrow 0+$ we have $f(t) \rightarrow \infty$ but, for all $t > 0$, the series in brackets in (3.5) converges. Again in this example we face cancellation problems and thus the range of t for which we can obtain accurate answers will be restricted. The exact value of $f(t)$ in this case is $(\pi t)^{-\frac{1}{2}} \cos 2\sqrt{at}$.

Example 3.4 $\bar{f}(s) = \ln s/(1+s)$.

This is quite different from the previous examples as we cannot expand $\ln s$ in terms of $1/s$. However, we can expand $\bar{f}(s)$ in the form

$$\bar{f}(s) = \frac{\ln s}{s} \left(1 - \frac{1}{s} + \frac{1}{s^2} - \frac{1}{s^3} + \cdots \right),$$

and from the table of transforms (Appendix §11.1) we find

$$\mathcal{L}^{-1} \left\{ \frac{\ln s}{s} \right\} = -\ln t - C,$$

where $C = 0.5772156649 \cdots$ is Euler's constant. Also,

$$\mathcal{L}^{-1} \left\{ \frac{\ln s}{s^n} \right\} = \frac{t^{n-1}}{\Gamma(n)} [\psi(n) - \ln t], \quad (n > 0),$$

where $\psi(n)$ is the Psi or Digamma function defined by

$$\psi(1) = -C, \quad \psi(n) = -C + \sum_{k=1}^{n-1} k^{-1}, \quad (n \geq 2).$$

Applying these results we obtain, after rearrangement and simplification,

$$f(t) = -e^{-t} \ln t + \sum_{n=0}^{\infty} \frac{(-t)^n \psi(n+1)}{(n)!}. \quad (3.6)$$

Example 3.5 $\bar{f}(s) = e^{-as} \bar{g}(s)$ where $\bar{g}(s) = \mathcal{L}\{g(t)\}$.

We know that $f(t) = H(t-a)g(t-a)$ and for $t \geq a$ we can proceed to get $g(t)$ as in previous examples and then replace t by $t-a$. Thus it follows from Example 3.2 equation (3.4) that if $\bar{f}(s) = e^{-as}/(s^2+1)$ we have

$$\begin{aligned} f(t) &= 0, & t < a, \\ &= (t-a) - \frac{(t-a)^3}{3!} + \frac{(t-a)^5}{5!} - \dots, & t \geq a. \end{aligned} \quad (3.7)$$

We conclude this section with an example which will be used in Chapter 9 to test the efficacy of various numerical methods of inversion.

Example 3.6 Determine a series expansion for $f(t)$ when

$$\bar{f}(s) = \frac{1}{s^{1/2} + s^{1/3}}.$$

We can write formally

$$\begin{aligned} \frac{1}{s^{1/2} + s^{1/3}} &= \frac{1}{s^{1/2}(1 + s^{-1/6})}, \\ &= \frac{1}{s^{1/2}} \left[1 - \frac{1}{s^{1/6}} + \frac{1}{s^{1/3}} - \dots + \frac{(-1)^n}{s^{n/6}} + \dots \right], \end{aligned}$$

and, using the result from §11.1,

$$\mathcal{L}^{-1} \left\{ \frac{1}{s^{\nu+1}} \right\} = \frac{t^{\nu}}{\Gamma(\nu+1)}, \quad \Re \nu > -1$$

we obtain

$$f(t) = t^{-1/2} \left[\frac{1}{\Gamma(\frac{1}{2})} - \frac{t^{1/6}}{\Gamma(\frac{2}{3})} + \frac{t^{1/3}}{\Gamma(\frac{5}{6})} - \dots + \frac{(-1)^n t^{n/6}}{\Gamma(\frac{n+3}{6})} + \dots \right]. \quad (3.8)$$

Thus when $t = 1$, for instance, we have

$$\begin{aligned} f(1) &= \left[\frac{1}{\Gamma(\frac{1}{2})} - \frac{1}{\Gamma(\frac{2}{3})} + \frac{1}{\Gamma(\frac{5}{6})} - \dots \right], \\ &= 0.23568175397 \dots \end{aligned}$$

3.1.1 An alternative treatment of series expansions

This approach was advocated by Chung and Sun [35] and others. It assumes that the function $f(t)$ can be written as

$$f(t) = \sum_0^n \alpha_i g_i(t), \quad (3.9)$$

where $g_i(t) = \exp(-it/k)$, k is a parameter and the α_i , $i = 0, 1, \dots, n$ are constants. This is equivalent to writing

$$f(t) = \alpha_0 + \alpha_1 z + \alpha_2 z^2 + \dots + \alpha_n z^n,$$

where $z = g_1(t)$. Since

$$\bar{f}(s) = \int_0^\infty f(t) e^{-st} dt,$$

we have

$$\bar{f}((j+1)/k) = \int_0^\infty f(t) e^{-t/k} g_j(t) dt,$$

we obtain a system of equations when we substitute $f(t)$ from (3.9) for $j = 0, 1, \dots, n$, namely,

$$\begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \cdots & \frac{1}{n+1} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \cdots & \frac{1}{n+2} \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \frac{1}{n+1} & \frac{1}{n+2} & \frac{1}{n+3} & \cdots & \frac{1}{2n+1} \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \cdots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} \bar{f}(1/k) \\ \bar{f}(2/k) \\ \cdots \\ \bar{f}((n+1)/k) \end{bmatrix}. \quad (3.10)$$

The main snag with using this approach is that the matrix in equation (3.10) is the well-known Hilbert matrix, which is known to be ill-conditioned. Thus, apart from the case where $f(t)$ exactly fits equation (3.9) for small n , we are unlikely to get very reliable results for the α_i and hence for $f(t)$. See Lucas [146].

3.2 Expansion in terms of Orthogonal Polynomials

In general, expansions in terms of orthogonal polynomials have superior convergence properties to those of power series expansions. One has only to think of the expansions for $1/(1+x)$ in $[0, 1]$

$$\frac{1}{1+x} = 1 - x + x^2 - x^3 + \dots, \quad (3.11)$$

and

$$\frac{1}{1+x} = \sqrt{2} \left(\frac{1}{2} T_0^*(x) + \lambda T_1^*(x) + \lambda^2 T_2^*(x) + \lambda^3 T_3^*(x) + \cdots \right), \quad (3.12)$$

where $\lambda = -3 + 2\sqrt{2}$ and $T_n^*(x)$ denotes the shifted Chebyshev polynomial of the first kind of degree n . Clearly (3.11) is not convergent in the ordinary sense when $x = 1$ (although it is convergent in the Cesaro sense) while (3.12) converges for all x in the range and also inside the ellipse with foci at $x = 0$ and $x = 1$ and semi-major axis $3/2$. It is thus quite natural to seek an approximation to $f(t)$ which has the form

$$f(t) = \sum_{k=0}^{\infty} a_k \phi_k(t), \quad (3.13)$$

where $\phi_k(t)$ is an appropriate orthogonal polynomial (or orthogonal function). This approach has been adopted by a number of researchers including Lanczos [124], Papoulis [164], Piessens [179], Bellman et al [16], etc.

3.2.1 Legendre Polynomials

Recall that

$$\bar{f}(s) = \int_0^{\infty} e^{-st} f(t) dt,$$

and make the substitution

$$x = e^{-\sigma t}, \quad (3.14)$$

where we assume $\sigma > 0$. Then

$$\begin{aligned} \bar{f}(s) &= \frac{1}{\sigma} \int_0^1 x^{(s/\sigma-1)} f(-\frac{1}{\sigma} \ln x) dx, \\ &= \frac{1}{\sigma} \int_0^1 x^{(s/\sigma-1)} g(x) dx, \quad \text{say.} \end{aligned}$$

Now let $s = (2r+1)\sigma$. Then

$$\bar{f}[(2r+1)\sigma] = \frac{1}{\sigma} \int_0^1 x^{2r} g(x) dx. \quad (3.15)$$

If we define $g(x)$ in $[-1, 0]$ by

$$g(-x) = g(x),$$

then $g(x)$ is an even function and can be expressed as a series of even Legendre polynomials. That is

$$g(x) = \sum_{k=0}^{\infty} \alpha_k P_{2k}(x), \quad (3.16)$$

or, equivalently,

$$f(t) = \sum_{k=0}^{\infty} \alpha_k P_{2k}(e^{-\sigma t}). \quad (3.17)$$

The problem facing us is “how do we determine the α_k ?”. First we note that since $P_{2k}(e^{-\sigma t})$ is an even polynomial of degree $2k$ in $e^{-\sigma t}$ and $\mathcal{L}\{e^{-2r\sigma t}\} = 1/(s + 2r\sigma)$ for $r = 0, 1, \dots, k$ we have

$$\bar{\phi}_{2k}(s) = \mathcal{L}\{P_{2k}(e^{-\sigma t})\} = \frac{A(s)}{s(s + 2\sigma) \cdots (s + 2k\sigma)}, \quad (3.18)$$

where $A(s)$ is a polynomial of degree $\leq k$. Further, because of the orthogonality of the Legendre polynomials,

$$\int_0^1 x^{2r} P_{2k}(x) dx = 0, \quad \text{for } r < k. \quad (3.19)$$

Hence, from (3.15) and (3.19), it follows that

$$\bar{\phi}_{2k}[(2r + 1)\sigma] = 0, \quad r = 0, 1, \dots, k - 1$$

and thus the roots of $A(s)$ are

$$(2r + 1)\sigma, \quad r = 0, 1, \dots, k - 1$$

and hence

$$\bar{\phi}_{2k}(s) = \frac{(s - \sigma)(s - 3\sigma) \cdots (s - (2k - 1)\sigma)}{s(s + 2\sigma) \cdots (s + 2k\sigma)} A,$$

where A is a constant. The initial value theorem gives

$$\lim_{s \rightarrow \infty} s \bar{\phi}_{2k}(s) = A = \lim_{t \rightarrow 0} P_{2k}(e^{-\sigma t}) = P_{2k}(1) = 1,$$

so that the Laplace transform of $P_{2k}(e^{-\sigma t})$ is

$$\bar{\phi}_{2k}(s) = \frac{(s - \sigma)(s - 3\sigma) \cdots [s - (2k - 1)\sigma]}{s(s + 2\sigma) \cdots (s + 2k\sigma)}. \quad (3.20)$$

The transform of equation (3.17) yields

$$\bar{f}(s) = \frac{\alpha_0}{s} + \sum_{k=1}^{\infty} \frac{(s - \sigma) \cdots [s - (2k - 1)\sigma]}{s \cdots (s + 2k\sigma)} \alpha_k. \quad (3.21)$$

Substituting in turn $s = \sigma, 3\sigma, \dots, (2k - 1)\sigma$ produces the triangular system of equations

$$\begin{aligned} \sigma \bar{f}(\sigma) &= \alpha_0 \\ \sigma \bar{f}(3\sigma) &= \frac{\alpha_0}{3} + \frac{2\alpha_1}{3 \cdot 5} \\ &\dots \\ \sigma \bar{f}((2k - 1)\sigma) &= \frac{\alpha_0}{2k - 1} + \frac{2k\alpha_1}{(2k - 1)(2k + 1)} + \cdots \\ &\quad + \frac{(2k - 2)(2k - 4) \cdots 2\alpha_{k-1}}{(2k - 1)(2k + 1) \cdots (4k - 1)} \end{aligned} \quad (3.22)$$

k	α_k
0	0.70710678
1	0.60394129
2	-0.56412890
3	0.45510745
4	-0.36389193
5	0.29225325
6	-0.23577693
7	0.19061806
8	-0.15396816
9	0.12382061
10	-0.09872863

Table 3.2: Coefficients in the Legendre expansion when $\bar{f}(s) = 1/\sqrt{s^2 + 1}$.

which can be solved sequentially.

Example 3.7 $\bar{f}(s) = 1/\sqrt{s^2 + 1}$.

Take $\sigma = 1$. Then, from (3.21), we have the system of equations

$$\begin{aligned} \frac{1}{\sqrt{2}} &= \alpha_0, \\ \frac{1}{\sqrt{10}} &= \frac{\alpha_0}{3} + \frac{2\alpha_1}{3 \cdot 5}, \\ \frac{1}{\sqrt{26}} &= \frac{\alpha_0}{5} + \frac{4\alpha_1}{5 \cdot 7} + \frac{4 \cdot 2\alpha_2}{5 \cdot 7 \cdot 9}, \quad \text{etc.,} \end{aligned}$$

which yields Table 3.2 .

It is clear from the table that the coefficients α_k decrease very slowly. The reason for this is that the function $g(x) = f(-\frac{1}{\sigma}|\log x|)$ is defined and expanded in a Legendre series on the interval $[-1, 1]$, but has a singularity at $x = 0$ inside the interval. This will be the case in general, even when $f(t)$ is well-behaved in $[0, \infty)$. This causes the Legendre series of $g(x)$ to converge slowly. Thus this method of inverting the Laplace transform is not very effective.

Additionally, because the coefficients on the diagonal decrease fairly rapidly, there is liable to be numerical instability in the determination of the α_k as k increases. To be more precise any error in α_0 could be magnified by a factor of about 4^k even if all other coefficients were computed exactly.

3.2.2 Chebyshev Polynomials

In the previous section we made the substitution $x = e^{-\sigma t}$ which transformed the interval $(0, \infty)$ into $(0, 1)$. Now we introduce the variable θ defined by

$$\cos \theta = e^{-\sigma t}, \quad (3.23)$$

which transforms the infinite interval to $(0, \pi/2)$ and $f(t)$ becomes

$$f\left(-\frac{1}{\sigma} \ln \cos \theta\right) = g(\theta), \quad \text{say.}$$

The defining formula for the Laplace transform now takes the form

$$\sigma \bar{f}(s) = \int_0^{\pi/2} (\cos \theta)^{(s/\sigma)-1} \sin \theta g(\theta) d\theta, \quad (3.24)$$

and by setting

$$s = (2k+1)\sigma, \quad k = 0, 1, 2, \dots$$

we have

$$\sigma \bar{f}[(2k+1)\sigma] = \int_0^{\pi/2} (\cos \theta)^{2k} \sin \theta g(\theta) d\theta. \quad (3.25)$$

For the convenience of representation we assume that $g(0) = 0$. (If this should not be the case we can arrange it by subtracting a suitable function from $g(\theta)$ — see Example 3.8). The function $g(\theta)$ can be expanded in $(0, \pi/2)$ as an odd-sine series

$$g(\theta) = \sum_{k=0}^{\infty} \alpha_k \sin(2k+1)\theta. \quad (3.26)$$

This expansion is valid in the interval $(-\pi/2, \pi/2)$. We now have to determine the coefficients α_k . Since

$$(\cos \theta)^{2k} \sin \theta = \left(\frac{e^{i\theta} + e^{-i\theta}}{2} \right)^{2k} \frac{e^{i\theta} - e^{-i\theta}}{2i},$$

expansion of the right hand side and collection of appropriate terms gives

$$\begin{aligned} 2^{2k} (\cos \theta)^{2k} \sin \theta &= \sin(2k+1)\theta + \dots + \left[\binom{2k}{r} - \binom{2k}{r-1} \right] \sin[2(k-r)+1]\theta \\ &+ \dots + \left[\binom{2k}{k} - \binom{2k}{k-1} \right] \sin \theta \end{aligned} \quad (3.27)$$

Substitution of (3.26) and (3.27) in (3.25) gives, because of the orthogonality of the odd sines in $(0, \pi/2)$ and

$$\int_0^{\pi/2} [\sin(2k+1)\theta]^2 d\theta = \frac{\pi}{4},$$

that

$$\begin{aligned} \sigma \bar{f}[(2k+1)\sigma] &= 2^{-2k} \frac{\pi}{4} \left\{ \left[\binom{2k}{k} - \binom{2k}{k-1} \right] \alpha_0 + \dots \right. \\ &\quad \left. + \left[\binom{2k}{r} - \binom{2k}{r-1} \right] \alpha_{k-r} + \dots + \alpha_k \right\}. \end{aligned}$$

Thus with $k = 0, 1, 2, \dots$ we get the triangular system of equations

$$\begin{aligned}
 \frac{4}{\pi} \sigma \bar{f}(\sigma) &= \alpha_0, \\
 2^2 \frac{4}{\pi} \sigma \bar{f}(3\sigma) &= \alpha_0 + \alpha_1, \\
 &\dots \quad \dots \quad \dots \\
 2^{2k} \frac{4}{\pi} \sigma \bar{f}[(2k+1)\sigma] &= \left[\binom{2k}{k} - \binom{2k}{k-1} \right] \alpha_0 + \dots \\
 &\quad + \left[\binom{2k}{r} - \binom{2k}{r-1} \right] \alpha_{k-r} + \dots + \alpha_k.
 \end{aligned} \tag{3.28}$$

The α_k are obtained from (3.28) by forward substitution and hence $g(\theta)$ can be obtained from (3.26). In practice one would only compute the first $N+1$ terms of (3.26), that is, the finite series

$$g_N(\theta) = \sum_{k=0}^N \alpha_k \sin(2k+1)\theta. \tag{3.29}$$

As $N \rightarrow \infty$ the function $g_N(\theta)$ tends to $g(\theta)$ with exact arithmetic. From a knowledge of $g(\theta)$ we can determine $f(t)$. Equation (3.26) can be written directly in terms of functions of t for if $x = \cos \theta$ and we define

$$U_{k-1}(x) = \frac{\sin k\theta}{\sin \theta},$$

where $U_k(x)$ is the Chebyshev polynomial of the second kind of degree k , then

$$\sin \theta = (1 - e^{-2\sigma t})^{1/2}$$

and

$$f(t) = (1 - e^{-2\sigma t})^{1/2} \sum_{k=0}^{\infty} \alpha_k U_{2k}(e^{-\sigma t}). \tag{3.30}$$

Example 3.8 $\bar{f}(s) = 1/\sqrt{s^2 + 1}$.

We shall take $\sigma = 1$ as in Example 3.7. Before we can start to determine the α_k we must check that $g(0) = 0$ or, equivalently, $f(0) = 0$. By the initial value theorem

$$f(0) = \lim_{s \rightarrow \infty} s f(s) = 1$$

so that a possible function we could employ to subtract from $f(t)$ would be the function 1. A more plausible function would be one having the same characteristics at ∞ . By the final value theorem

$$\lim_{t \rightarrow \infty} f(t) = \lim_{s \rightarrow 0} s f(s) = 0.$$

A function which takes the value 1 at $t = 0$ and tends to zero as $t \rightarrow \infty$ is e^{-t} and therefore we shall work with the function $F(t) = f(t) - e^{-t}$ as $F(0) = 0$

k	α_k
0	0.26369654
1	0.07359870
2	-0.14824954
3	0.09850917
4	-0.07693976
5	0.05470060
6	-0.04226840
7	0.03102729
8	-0.02397057
9	0.01764179
10	-0.01340272

Table 3.3: Coefficients in the Chebyshev expansion when $\bar{f}(s) = 1/\sqrt{s^2 + 1}$.

and the corresponding $G(0) = 0$. Since $\bar{F}(s) = \bar{f}(s) - 1/(s+1)$ the equations for α_k are, from equation (3.28),

$$\begin{aligned}
\frac{4}{\pi} \left(\frac{1}{\sqrt{2}} - \frac{1}{2} \right) &= \alpha_0, \\
2^2 \frac{4}{\pi} \left(\frac{1}{\sqrt{10}} - \frac{1}{4} \right) &= \alpha_0 + \alpha_1, \\
2^4 \frac{4}{\pi} \left(\frac{1}{\sqrt{26}} - \frac{1}{6} \right) &= 2\alpha_0 + 3\alpha_1 + \alpha_2, \\
2^6 \frac{4}{\pi} \left(\frac{1}{\sqrt{50}} - \frac{1}{8} \right) &= 5\alpha_0 + 9\alpha_1 + 5\alpha_2 + \alpha_3, \quad \text{etc.}
\end{aligned}$$

Solution of these equations yields Table 3.3 . Now the coefficients along the main diagonal are all 1, so we do not have the same problem as in the previous section of diagonal elements decreasing rapidly, but decimal digits can be lost in the computation because of cancellation brought about by the large coefficients.

Lanczos [124] has a slightly different approach using the shifted Chebyshev polynomials $U_k^*(x)$.

3.2.3 Laguerre Polynomials

In this approach we attempt to approximate the function $f(t)$ by an expansion of the form

$$f(t) = \sum_{k=0}^{\infty} \alpha_k \phi_k(t), \quad (3.31)$$

where

$$\phi_k(t) = e^{-t} L_k(t), \quad (3.32)$$

and $L_k(t)$ is the Laguerre polynomial of degree k which is defined by

$$L_k(t) = e^t \frac{d^k}{dt^k} \left[\frac{e^{-t} t^k}{k!} \right]. \quad (3.33)$$

Now we know that the Laplace transform of $\phi_k(t)$ is given by

$$\bar{\phi}_k(s) = \frac{s^k}{(s+1)^{k+1}},$$

so that the Laplace transform of equation (3.31) is

$$\bar{f}(s) = \sum_{k=0}^{\infty} \alpha_k \frac{s^k}{(s+1)^{k+1}}. \quad (3.34)$$

For small s the binomial expansion for $s^k/(s+1)^{k+1}$ is

$$\frac{s^k}{(s+1)^{k+1}} = s^k \sum_{r=0}^{\infty} \binom{r+k}{k} (-1)^r s^r. \quad (3.35)$$

Expansion of $\bar{f}(s)$ about the origin gives

$$\bar{f}(s) = \sum_{k=0}^{\infty} \beta_k s^k. \quad (3.36)$$

Thus, combining equations (3.34), (3.35) and (3.36) and equating powers of s , we have

$$\begin{aligned} \beta_0 &= \alpha_0, \\ \beta_1 &= \alpha_1 - \alpha_0, \\ \dots &\dots \dots \\ \beta_k &= \alpha_k - \binom{k}{1} \alpha_{k-1} + \dots + (-1)^k \alpha_0. \end{aligned} \quad (3.37)$$

For this triangular system of equations we can obtain an explicit formula for each α_k , namely

$$\alpha_k = \beta_k + \binom{k}{1} \beta_{k-1} + \dots + \binom{k}{r} \beta_{k-r} + \dots + \beta_0. \quad (3.38)$$

Clearly, if k has even moderate value, the coefficients in the above formula can be quite substantial if all the β_k are positive but, hopefully, since $L_k(t)$ satisfies the inequality

$$|L_k(t)| \leq e^{t/2}, \quad t \geq 0,$$

this will not result in a divergent series.

k	α_k
0	1.00000000
1	1.00000000
2	0.50000000
3	-0.50000000
4	-1.62500000
5	-2.12500000
6	-1.18750000
7	1.43750000
8	4.77343750
9	6.46093750
10	3.68359375

Table 3.4: Coefficients in the Laguerre expansion when $\bar{f}(s) = 1/\sqrt{s^2 + 1}$.

n	$\sigma = 0.5$	$\sigma = 1.0$
15	0.2109	0.2155
20	0.2214	0.2185
25	0.2255	0.2339

Table 3.5: Estimation of $J_0(2)$ using Legendre expansion.

Example 3.9 $\bar{f}(s) = 1/\sqrt{s^2 + 1}$.

The first task is to determine the β_k . By expanding $(s^2 + 1)^{-1/2}$ we have

$$(s^2 + 1)^{-1/2} = 1 - \frac{1}{2}s^2 + \frac{3}{8}s^4 - \frac{5}{16}s^6 + \cdots + \left(\frac{-1}{4}\right)^n \binom{2n}{n} s^{2n} + \cdots.$$

Thus, from (3.37),

$$\begin{aligned} \alpha_0 &= 1, \\ \alpha_1 &= 1, \\ \alpha_2 &= 1/2, \quad \text{etc.} \end{aligned}$$

we obtain Table 3.4 .

In the above we have outlined the method for determining the coefficients in the various expansions but have not commented on their effectiveness. In Table 3.5 we have used the truncated series (3.22) to estimate the value of $J_0(2) = 0.22389$ using two values of σ and various values of n the number of terms of the series employed. Clearly this is not very efficient and we are not doing as well here as we did in §3.1. Similar results are obtained when we expand in terms of other orthogonal polynomials. However, if we use orthonormal Laguerre functions, which was the approach adopted by Weeks [247], we are more successful.

3.2.4 The method of Weeks

This method incorporates the ideas of Papoulis and Lanczos. We attempt to obtain a series expansion for $f(t)$ in terms of the orthonormal Laguerre functions

$$\Phi_k(t) = e^{-t/2} L_k(t), \quad k = 0, 1, 2, \dots \quad (3.39)$$

where $L_k(t)$ is the Laguerre polynomial of degree k . Thus

$$\int_0^\infty \Phi_k(t) \Phi_\ell(t) dt = \begin{cases} 0 & \text{if } k \neq \ell \\ 1 & \text{if } k = \ell \end{cases} \quad (3.40)$$

$$\Phi_k(0) = 1. \quad (3.41)$$

Any function $f(t)$ satisfying the conditions (1.2) and §2.5 can be approximated by a function $f_N(t)$ such that

$$f_N(t) = e^{ct} \sum_{k=0}^N a_k \Phi_k\left(\frac{t}{T}\right), \quad (3.42)$$

where $T > 0$ is a scale factor and

$$a_k = \frac{1}{T} \int_0^\infty e^{-ct} f(t) \Phi_k\left(\frac{t}{T}\right) dt. \quad (3.43)$$

The function $f_N(t)$ approximates $f(t)$ in the sense that, for any $\epsilon > 0$, there exists an integer N_0 such that

$$\int_0^\infty e^{-2ct} |f(t) - f_N(t)|^2 dt < \epsilon \quad (3.44)$$

whenever $N > N_0$.

Now suppose $\bar{f}_N(s)$ is the Laplace transform of $f_N(t)$, i.e.,

$$\begin{aligned} \bar{f}_N(s) &= \int_0^\infty e^{-st} f_N(t) dt, \\ &= \int_0^\infty e^{-(s-c)t} \sum_{k=0}^N a_k \Phi_k\left(\frac{t}{T}\right) dt, \\ &= \sum_{k=0}^N a_k \int_0^\infty e^{-(s-c)t} e^{-\frac{1}{2}t/T} L_k\left(\frac{t}{T}\right) dt, \\ &= \sum_{k=0}^N a_k \frac{(s - c - \frac{1}{2T})^k}{(s - c + \frac{1}{2T})^{k+1}} \end{aligned} \quad (3.45)$$

On the line $s = c$ in the complex plane $\bar{f}_N(c + i\omega)$ converges in the mean to $\bar{f}(c + i\omega)$ with increasing N . This result is a consequence of Parseval's theorem (Chapter 2) in the form

$$\int_0^\infty e^{-2ct} |f(t) - f_N(t)|^2 dt = \frac{1}{2\pi} \int_{-\infty}^\infty |\bar{f}(c + i\omega) - \bar{f}_N(c + i\omega)|^2 d\omega. \quad (3.46)$$

For, since $f(t) - f_N(t)$ satisfies the required condition of being $O(e^{\gamma t})$ if $c > \gamma$ we have by comparison with (3.44) that given any $\epsilon > 0$, $\exists N$ such that

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} |\bar{f}(c + i\omega) - \bar{f}_N(c + i\omega)|^2 d\omega < \epsilon, \quad (3.47)$$

whenever $N > N_0$ and this establishes the result.

Whereas Papoulis determined the a_k by a Taylor series expansion, Weeks finds a trigonometric expansion of the Laplace transform. If $s = c + i\omega$ then substitution of (3.45) into (3.47) gives

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \left| \bar{f}(c + i\omega) - \sum_{k=0}^N a_k \frac{(i\omega - \frac{1}{2T})^k}{(i\omega + \frac{1}{2T})^{k+1}} \right|^2 d\omega < \epsilon, \quad (3.48)$$

whenever $N > N_0$. Next we make the change of variable

$$\omega = \frac{1}{2T} \cot \frac{1}{2}\theta,$$

and note the identities

$$\frac{i \cos \frac{1}{2}\theta - \sin \frac{1}{2}\theta}{i \cos \frac{1}{2}\theta + \sin \frac{1}{2}\theta} = e^{i\theta},$$

$$|i \cos \frac{1}{2}\theta + \sin \frac{1}{2}\theta|^2 = 1,$$

to obtain

$$\frac{T}{2\pi} \left\{ \left(\int_{-\pi}^{0-} + \int_{0+}^{\pi} \right) \left| \left(\frac{1}{2T} + \frac{i}{2T} \cot \frac{1}{2}\theta \right) \bar{f}(c + \frac{i}{2T} \cot \frac{1}{2}\theta) - \sum_{k=0}^N a_k e^{ik\theta} \right|^2 d\theta < \epsilon, \right. \quad (3.49)$$

whenever $N > N_0$. The inequality (3.49) implies that

$$\left(\frac{1}{2T} + \frac{i}{2T} \cot \frac{1}{2}\theta \right) \bar{f}(c + \frac{i}{2T} \cot \frac{1}{2}\theta) \approx \sum_{k=0}^N a_k e^{ik\theta}, \quad (3.50)$$

in the sense that the right hand side of (3.50) converges in the mean to the left hand side as N increases. If

$$\bar{f}(s) = G + iH, \quad (3.51)$$

where G and H are real and we take the real part of equation (3.50) we have

$$A(\theta) = \frac{1}{2T} (G - H \cot \frac{1}{2}\theta) \approx \sum_{k=0}^N a_k \cos k\theta. \quad (3.52)$$

The coefficients a_k can then be approximated by trigonometric interpolation

$$a_0 = \frac{1}{N+1} \sum_{j=0}^N A(\theta_j), \quad (3.53)$$

$$a_k = \frac{2}{N+1} \sum_{j=0}^N A(\theta_j) \cos k\theta_j, \quad k > 0 \quad (3.54)$$

where

$$\theta_j = \left(\frac{2j+1}{N+1} \right) \frac{\pi}{2}. \quad (3.55)$$

We now consider some practicalities. From the analysis in Appendix 11.6, if x_k is the largest zero of the equation $L_k(x) = 0$ then x_k satisfies the inequality

$$x_k \leq 4k - 6, \quad k \geq 4$$

(see Cohen [45]). Thus the function $\Phi_k(t)$ oscillates in the interval $0 < t < 4k - 6$ and approaches zero monotonically for $t > 4k - 6$. Hence, intuitively, one would only expect oscillatory functions to be representable by a linear combination of the Φ 's in the interval $(0, t_{\max})$ where

$$\frac{t_{\max}}{T} < 4N - 6.$$

Weeks states, on the basis of empirical evidence, that a satisfactory choice of the parameter T is obtained by taking

$$T = \frac{t_{\max}}{N}. \quad (3.56)$$

With this choice of T , (3.42) gives a good approximation to $f(t)$ in $(0, t_{\max})$ provided c is properly chosen and N is sufficiently large. If $\Re s = \gamma_0$ marks the position of the line through the right-most singularity then Weeks suggests a suitable value of c is

$$c = \gamma_0 + 1/t_{\max}.$$

Once γ_0 has been determined and a value of t_{\max} assigned then a value of N has to be chosen. Weeks [247] took values between 20 and 50. T now follows from (3.56) and the a_k can be estimated from (3.53) - (3.55). $f_N(t)$ is then readily determined from (3.42) by noting that the $\Phi_k(t)$ satisfy the recurrence relations

$$\begin{aligned} \Phi_0(t) &= e^{-\frac{1}{2}t}, \\ \Phi_1(t) &= (1-t)\Phi_0(t), \\ k\Phi_k(t) &= (2k-1-t)\Phi_{k-1}(t) - (k-1)\Phi_{k-2}(t), \quad k > 1. \end{aligned}$$

Weeks, op cit., also makes additional points relating to the computation of the terms $\cos \theta_j$ and $A(\theta_j)$.

Subsequently, Weeks's method has been investigated by Lyness and Giunta [150] and has been modified by using the Cauchy integral representation for the derivative. Thus if we write

$$f(t) = e^{ct} \sum_{k=0}^{\infty} a_k e^{-bt/2} L_k(bt), \quad (3.57)$$

then b corresponds to $1/T$ in the Weeks method. If we define

$$\psi(z) = \frac{b}{1-z} \bar{f} \left(\frac{b}{1-z} - \frac{b}{2} + c \right) \quad (3.58)$$

then $\psi(z)$ is a regular function inside a circle $|z| < R$ with $R \geq 1$. Moreover, the coefficients a_k in (3.57) are exactly the coefficients in the Taylor expansion of $\psi(z)$, viz.,

$$\psi(z) = \sum_{k=0}^{\infty} a_k z^k. \quad (3.59)$$

Hence

$$a_k = \frac{\psi^{(k)}(0)}{k!} = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{\psi(z)}{z^{k+1}} dz, \quad (3.60)$$

where \mathcal{C} could be any contour which includes the origin and does not contain any singularity of $\psi(z)$ but which we shall take to be a circle of radius r centre the origin ($r < R$). Thus

$$a_k = \frac{1}{2\pi i} \int_{|z|=r} \frac{\psi(z)}{z^{k+1}} dz = \frac{1}{2\pi r^k} \int_0^{2\pi} \psi(re^{i\theta}) e^{-ik\theta} d\theta, \quad k \geq 0. \quad (3.61)$$

It is convenient to approximate the integral by means of an m -point trapezium rule where m is even. That is, by

$$a_k(T_m, r) = \frac{1}{r^k m} \sum_{j=1}^m \psi(re^{2\pi i j/m}) e^{-2\pi i k j/m}. \quad (3.62)$$

Now $\psi(z)$ is real when z is real and $\psi(\bar{z}) = \overline{\psi(z)}$ so that the sum in (3.62) requires only $m/2$ independent evaluations of (both the real and imaginary parts of) $\psi(z)$. Thus we obtain the Lyness and Giunta modification to Weeks's method

$$\begin{aligned} a_k(T_m, r) &= \frac{2}{r^k m} \sum_{j=1}^{m/2} \Re(\psi(re^{2\pi i j/m})) \cos(2\pi k j/m) \\ &\quad + \frac{2}{r^k m} \sum_{j=1}^{m/2} \Im(\psi(re^{2\pi i j/m})) \sin(2\pi k j/m), \end{aligned} \quad (3.63)$$

for values of k from 0 to $m-1$. Here $m-1$ corresponds to the N of Weeks and the function $f_N(t)$ would be our approximation to $f(t)$.

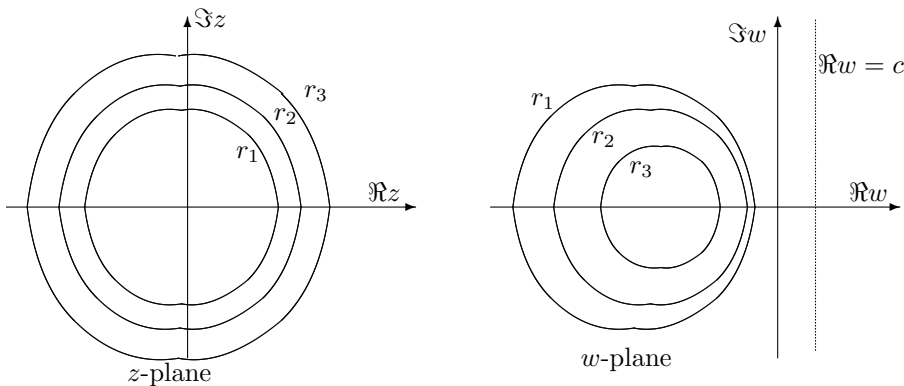


Figure 3.1: The transformation (3.64), $r > 1$.

The method we have described depends crucially on the choice of the free parameters b and c . The parameters have to a large extent been chosen by rule of thumb. Giunta et al [97] look at the problem of finding the optimal b for a given c for a restricted class of transforms \mathcal{A} . However, they did not engage in determining c and relied on a priori knowledge of the singularities. A FORTRAN program for Weeks's method based on the paper by Garbow et al [91] can be found at the website

www.cf.ac.uk/maths/cohen/programs/inverselaplace/transform/ .

Weideman [248] presents two methods for determining b and c . The first assumes that the theory of Giunta et al is applicable while the second is more general.

Weideman notes that the transformation

$$w = c + \frac{b}{1-z} - \frac{1}{2}b, \quad (3.64)$$

which occurs in (3.59), maps circles of radius r centered at the origin of the z -plane to circles with radius $2b'r/|r^2 - 1|$ and centre $c - b'(r^2 + 1)/(r^2 - 1)$ in the w -plane, where $b' = b/2$. In particular the interiors of concentric circles in the z -plane with $r > 1$ are mapped into the exteriors of circles in the w -plane and vice versa. If $r < 1$ then the image circles lie in the half-plane $\Re w > c$ — see Figure 3.1. As Weideman points out the image circles corresponding to radii r and $1/r$ are mirror images in the line $\Re w = c$ and this line corresponds to the image of the unit circle. This informs us that the radius of convergence of the Maclaurin series (3.59) satisfies $R \geq 1$.

Weideman applies the Cauchy estimate to the integral (3.60) to show that

$$|a_k| \leq \frac{\kappa(r)}{r^k}, \quad k = 0, 1, 2, \dots \quad (3.65)$$

where $\kappa(r) = \max_{|z|=r} |\psi(z)|$, to infer that for the class of transforms in \mathcal{A} the coefficients a_k decay exponentially. An example of a transform not in \mathcal{A} is $\tilde{f}(s) = 1/\sqrt{s}$. Lyness and Giunta chose $r < 1$ in (3.61) but Weideman takes $r = 1$ and instead of using the trapezium rule which would require $\theta = 0$ and $\theta = 2\pi$, i.e. $z = 1$ which corresponds to $w = \infty$ being involved in the summation, he uses the equally accurate mid-point rule which avoids the singular point. Thus \tilde{a}_k , the approximation to a_k is given by

$$\tilde{a}_k = \frac{e^{-ikh/2}}{2N} \sum_{j=-N}^{N-1} \psi(e^{i\theta_{j+1/2}}) e^{-ik\theta_j}, \quad k = 0, \dots, N-1, \quad (3.66)$$

where $\theta_j = jh$, $h = \pi/N$. Weideman computed this as a FFT (fast Fourier transform) of length $2N$ and notes that only the a_k , $0 \leq k \leq N-1$, are used in evaluating (3.57).

The actual expression employed in estimating $f(t)$ is

$$\tilde{f}(t) = e^{ct} \sum_{k=0}^{N-1} \tilde{a}_k (1 + \epsilon_k) e^{-bt/2} L_k(bt), \quad (3.67)$$

where ϵ_k denotes the relative error in the floating point representation of the computed coefficients, i.e., $\text{fl}(\tilde{a}_k) = (\tilde{a}_k)(1 + \epsilon_k)$. Subtracting (3.67) from (3.57), assuming $\sum_{k=0}^{\infty} |a_k| < \infty$, we obtain

$$|f(t) - \tilde{f}(t)| \leq e^{ct}(T + D + C),$$

where

$$T = \sum_{k=N}^{\infty} |a_k|, \quad D = \sum_{k=0}^{N-1} |a_k - \tilde{a}_k|, \quad C = \epsilon \sum_{k=0}^{N-1} |\tilde{a}_k|,$$

are respectively the truncation, discretization and conditioning error bounds. ϵ is the machine round-off unit so that for each k , $|\epsilon_k| \leq \epsilon$. Since it can be shown that

$$\tilde{a}_k - a_k = \sum_{j=1}^{\infty} (-1)^j a_{k+2jN}, \quad k = 0, 1, \dots, N-1$$

this yields

$$D = \sum_{k=0}^{N-1} |a_k - \tilde{a}_k| \leq \sum_{k=0}^{N-1} \sum_{j=1}^{\infty} |a_{k+2jN}|.$$

The dominant term on the right hand side is $|a_{2N}|$ and thus D is negligible compared with T which has leading term $|a_N|$, because Weideman opts for the FFT method for evaluating the summation. This is not the case in the

Lyness-Giunta formulation where the truncation and discretization errors are of comparable magnitude. Thus basically the error in $f(t)$ will be minimized if we can determine the optimal c and b (or b') to minimize

$$E = e^{ct} \left(\sum_{k=N}^{\infty} |a_k| + \epsilon \sum_{k=0}^{N-1} |a_k| \right). \quad (3.68)$$

Here the tilde has been dropped since the algorithms cannot distinguish between true and computed coefficients.

For transforms in the class \mathcal{A} we can employ the Cauchy estimate (3.65) to bound the truncation and conditioning errors giving

$$T = \sum_{k=N}^{\infty} |a_k| \leq \frac{\kappa(r)}{r^N(r-1)}, \quad C = \epsilon \sum_{k=0}^{N-1} |a_k| \leq \epsilon \frac{r\kappa(r)}{r-1}, \quad (3.69)$$

which is valid for each $r \in (1, R)$. Inserting these two bounds into (3.68) we have an error estimate in terms of r which we can try and minimize as a function of c and b (or b').

Weideman remarks that while he has had some success with the above approach for estimating the optimal parameters the Cauchy estimates are fine for a_k when k is large but not so effective for intermediate values. He adds that provided r is selected judiciously the bound for T in (3.69) is tight but this might not be the case for C , whatever the choice of r .

To obtain his first algorithm he assumes that the transform belongs to the class \mathcal{A} and has finitely many singularities at s_1, s_2, \dots, s_m which may be either poles or branch points and is assumed to be real or occur as complex conjugate pairs. It follows from (3.69), or the work of Giunta et al, that T is minimized if R is maximized. For given $c > \gamma$ the optimal b' is thus given by

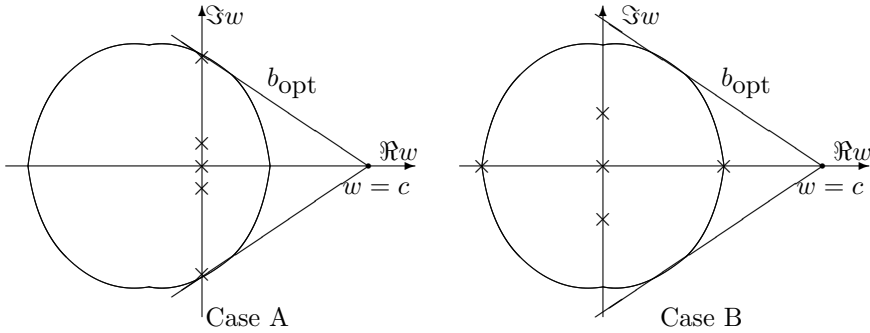
$$R(b'_{\text{opt}}) = \max_{b' > 0} R(b'). \quad (3.70)$$

Giunta et al gave the following geometric description of b'_{opt} . For fixed $c > \gamma$ consider the family of circles, parameterized by b' which contain all the singularities of $\tilde{f}(w)$ — see Figs. 3.1 and 3.2. If we imagine two tangent lines drawn from the point $w = c$ to each circle and we select the circle in this family which minimizes the angle between the two tangent lines then the optimal value of b' is the length of the tangent segment from the point $w = c$ to the optimal circle. Two cases have to be considered:-

Case A. The optimal circle is determined by a complex conjugate pair of singularities s_j and \bar{s}_j and only occurs if the tangents to the circle through $w = c$ pass through $w = s_j$ and $w = \bar{s}_j$.

Case B. The optimal circle passes through two distinct pairs (s_j, \bar{s}_j) and (s_k, \bar{s}_k) which includes the case where s_j and s_k are real.

Weideman now determines the critical curve in the (c, b') plane on which the optimal point is located.

Figure 3.2: Geometric significance of b_{opt} .

If Case A appertains he denotes the critical singularities which determine the optimal circle by $s = \alpha \pm i\beta$ and finds

$$R = \left| \frac{s - c - b'}{s - c + b'} \right| = \left| \frac{(\alpha - c - b')^2 + \beta^2}{(\alpha - c + b')^2 + \beta^2} \right|^{1/2}.$$

To satisfy (3.70) we require $\partial R / \partial b' = 0$ which yields the hyperbola

$$b'^2 - (c - \alpha)^2 = \beta^2. \quad (3.71)$$

Likewise for Case B if the two critical singularities are $s_1 = \alpha_1 + i\beta_1$ and $s_2 = \alpha_2 + i\beta_2$, where $\alpha_1 \neq \alpha_2$, both singularities correspond to the same value of R and thus

$$\left| \frac{s_1 - c - b'}{s_1 - c + b'} \right| = \left| \frac{s_2 - c - b'}{s_2 - c + b'} \right|.$$

This also yields a hyperbola

$$b'^2 - c^2 + \frac{|s_2|^2 - |s_1|^2}{\alpha_2 - \alpha_1} c + \frac{\alpha_2 |s_1|^2 - \alpha_1 |s_2|^2}{\alpha_2 - \alpha_1} = 0. \quad (3.72)$$

This provides the basis for the algorithms. Weideman replaces E in (3.68) by

$$E(c, b') = e^{ct} \left(\sum_{k=N}^{2N-1} |a_k| + \epsilon \sum_{k=0}^{N-1} |a_k| \right), \quad (3.73)$$

which can be computed by a FFT of length $4N$. For the cases where the Weeks method is suitable this truncation is fairly inconsequential because of the rapid decay of the a_k . We have

ALGORITHM 1($\bar{f} \in \mathcal{A}$) Given t, N and an interval $[c_0, c_{\max}]$ that is likely to contain the optimal c and b' defined by (3.71) or (3.72) the algorithm solves

$$c = \{c \in [c_0, c_{\max}] \mid E(c, b') = \text{a minimum}\}. \quad (3.74)$$

When $\bar{f} \notin \mathcal{A}$ the above theory does not apply and the optimal curve for b' has to be determined numerically. A good approximation to this curve is determined by the value of b' that minimizes the truncation error estimate for any $c > c_0$. We now compute b' from

$$b'(c) = \{b' > 0 \mid T(c, b') = \text{a minimum}\}$$

where

$$T(c, b') = \sum_{k=N}^{2N-1} |a_k|.$$

ALGORITHM 2($\bar{f} \notin \mathcal{A}$) Given t, N and a rectangle $[c_0, c_{\max}] \times [0, b'_{\max}]$ that is likely to contain the optimal (c, b') the algorithm solves the nested problem

$$c = \{c \in [c_0, c_{\max}] \mid E(c, b') = \text{a minimum}\}, \quad (3.75)$$

where

$$b'(c) = \{b' \in [0, b'_{\max}] \mid T(c, b') = \text{a minimum}\}. \quad (3.76)$$

Weideman found that Brent's algorithm [23], which combines a golden section search with successive parabolic interpolation, worked well as a minimization technique for (3.74) - (3.76) but that the quantities minimized were $\ln E$ and $\ln T$ because of the smallness of E and T . He points out that the two algorithms assume a fixed value of t . If $f(t)$ is to be computed at many t values, $t \in [0, t_{\max}]$, then if N is large the optimal values (c, b') are virtually independent of t and the optimal point is determined by a balance between the quantities T and C (both independent of t). For intermediate N one should take $t = t_{\max}$ which should correspond to the largest absolute error in the Weeks expansion. Details of numerical tests are available in Weideman's paper and a MATLAB file of his paper is available via electronic mail from weideman@na-net.ornl.gov.

3.3 Multi-dimensional Laplace transform inversion

A number of authors have attempted to invert multi-dimensional Laplace transforms and, in particular, two dimensional Laplace transforms. Essentially, their methods are a concatenation of 1-dimensional methods. Included among them are the methods of Moorthy [157] and Abate et al [1] who have extended the

Weeks method. The latter use an expansion in terms of Laguerre polynomials $\Phi_k(t)$ which takes the form

$$f(t_1, t_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} q_{m,n} \Phi_m(t_1) \Phi_n(t_2), \quad t_1, t_2 \geq 0, \quad (3.77)$$

where, as earlier,

$$\Phi_k(t) = e^{-t/2} L_k(t), \quad t \geq 0,$$

and

$$\begin{aligned} Q(z_1, z_2) &\equiv \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} q_{m,n} z_1^m z_2^n \\ &= (1 - z_1)^{-1} (1 - z_2)^{-1} \bar{f} \left(\frac{1 + z_1}{2(1 - z_1)}, \frac{1 + z_2}{2(1 - z_2)} \right), \end{aligned} \quad (3.78)$$

is the Laguerre generating function and $z_i = (2s_i - 1)/(2s_i + 1)$, $i = 1, 2$ and the Laplace transform exists for $\Re s_1, \Re s_2 > 0$. The functions $\Phi_m(t_1)$ and $\Phi_n(t_2)$ are computed from the one-dimensional recurrence relation

$$\Phi_k(t) = \left(\frac{2k - 1 - t}{k} \right) \Phi_{k-1}(t) - \left(\frac{k - 1}{k} \right) \Phi_{k-2}(t), \quad (3.79)$$

where $\Phi_0(t) = e^{-t/2}$ and $\Phi_1(t) = (1 - t)e^{-t/2}$. The Laguerre functions $\Phi_k(t)$ tend to zero slowly as $k \rightarrow \infty$ and hence, for an effective algorithm, we must have $q_{m,n}$ decaying at an appreciable rate as either m or n gets large. If this does not happen then Abate et al use scaling or summation acceleration.

From (3.78) the computation of $q_{m,n}$ requires the double inversion of the bivariate generating function $Q(z_1, z_2)$ and this was achieved by applying a Fourier series based inversion algorithm given in Choudhury et al [34]. By modifying equation (3.5) in that paper Abate et al obtain the approximation

$$\begin{aligned} q_{m,n} \approx \bar{q}_{m,n} &\equiv \frac{1}{m_1 r_1^m} \{ \Re[\hat{Q}(r_1, n)] + (-1)^m \Re[\hat{Q}(-r_1, n)] \} \\ &+ \sum_{k=1}^{(m_1/2)-1} \Re[e^{(-2\pi i k m / m_1)} \hat{Q}(r_1 e^{2\pi i k / m_1}, n)], \end{aligned} \quad (3.80)$$

and

$$\hat{Q}(z_1, n) = \frac{1}{m_2 r_2^n} \sum_{k=-m_2/2}^{(m_2/2)-1} e^{(-2\pi i k n / m_2)} Q(z_1, r_2 e^{2\pi i k / m_2}). \quad (3.81)$$

The resulting aliasing error, E , is given by

$$E = \bar{q}_{m,n} - q_{m,n} = \sum_{\substack{j=0 \\ j+k>0}}^{\infty} \sum_{k=0}^{\infty} q_{m+jm_1, n+km_2} r_1^{jm_1} r_2^{km_2}.$$

If $|q_{m+jm_1, n+km_2}| \leq C$ for each j, k and r_1, r_2 are chosen so that

$$r_1 = 10^{-A_1/m_1}, \quad r_2 = 10^{-A_2/m_2}$$

then it can be shown that

$$|E| \leq \frac{C(10^{-A_1} + 10^{-A_2})}{(1 - 10^{-A_1})(1 - 10^{-A_2})} \approx C(10^{-A_1} + 10^{-A_2}).$$

The aliasing error can thus be controlled by choosing A_1 and A_2 large, provided C is not large. Typical values chosen by Abate et al were $A_1 = 11$ and $A_2 = 13$. In order to effect the inversion using the FFT, m_1 and m_2 were chosen so that

$$m_1 = 2\ell_1 M, \quad m_2 = 2\ell_2 N$$

and, for example, $M = 128$, $\ell_1 = 1$, $N = 64$, $\ell_2 = 2$ giving $m_1 = m_2 = 256$. Next (3.80) and (3.81) are rewritten as

$$\bar{q}_{m,n} = \frac{1}{m_1 r_1^m} \sum_{k=0}^{m_1-1} e^{-2\pi i k m / m_1} \hat{Q}(r_1 e^{2\pi i k / m_1}, n), \quad (3.82)$$

$$\hat{Q}(z_1, n) = \frac{1}{m_2 r_2^n} \sum_{k=0}^{m_2-1} e^{-2\pi i k n / m_2} Q(z_1, r_2 e^{2\pi i k / m_2}). \quad (3.83)$$

If we define the $(m_1 \times m_2)$ dimensional sequences $\{a_{m,n}\}$ and $\{b_{m,n}\}$ over $0 \leq m \leq m_1 - 1$ and $0 \leq n \leq m_2 - 1$ by

$$a_{m,n} = \bar{q}_{m,n} r_1^m r_2^n, \quad (3.84)$$

$$b_{m,n} = Q(r_1 e^{2\pi i m / m_1}, r_2 e^{2\pi i n / m_2}), \quad (3.85)$$

and note that $a_{m,n}$ and $\bar{q}_{m,n}$ are only defined in the range $0 \leq m \leq M - 1$, $0 \leq n \leq N - 1$ we can extend the definition over the full range by means of the inverse discrete Fourier transform (IDFT) relation

$$a_{m,n} = \frac{1}{m_1 m_2} \sum_{j=0}^{m_1-1} \sum_{k=0}^{m_2-1} \exp\left(-\frac{2\pi i j m}{m_1} - \frac{2\pi i k n}{m_2}\right) b_{j,k}, \quad (3.86)$$

which follows from (3.82) and (3.83).

Equation (3.86) implies that $\{b_{m,n}\}$ is the two-dimensional DFT of $\{a_{m,n}\}$ and conversely $\{a_{m,n}\}$ is the two-dimensional IDFT of $\{b_{m,n}\}$. First the $\{b_{m,n}\}$ are computed from (3.85) and stored. Then the $a_{m,n}$ are computed using any standard two-dimensional FFT algorithm. Finally, the $\bar{q}_{m,n}$ are obtained from (3.84). Fuller details of the procedure can be found in [1].

Moorthy's approach is to extend the one dimensional methods of Weeks and Piessens and Branders [182] but to use an expansion in terms of the generalised

Laguerre polynomials $L_n^{(\alpha)}(t)$. He assumes that we can express $f(t_1, t_2)$ in the form

$$f(t_1, t_2) = t_1^{\alpha_1} t_2^{\alpha_2} e^{c_1 t_1 + c_2 t_2} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} q_{m,n} L_m^{\alpha_1}(bt_1) L_n^{\alpha_2}(bt_2), \quad (3.87)$$

where $-1 < \alpha_1, \alpha_2 < 1$ and $b > 0$. If $\bar{f}(s_1, s_2)$ is the Laplace transform of $f(t_1, t_2)$ where $\Re s_1 > c_1$ and $\Re s_2 > c_2$ then it follows from (3.87) that

$$\begin{aligned} \bar{f}(s_1, s_2) &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} q_{m,n} \frac{\Gamma(m + \alpha_1 + 1) \Gamma(n + \alpha_2 + 1)}{m! n!} \\ &\quad \times \frac{(s_1 - c_1 - b)^m}{(s_1 - c_1)^{m+1}} \frac{(s_2 - c_2 - b)^n}{(s_2 - c_2)^{n+1}}. \end{aligned} \quad (3.88)$$

If we set

$$z_1 = \frac{(s_1 - c_1 - b)}{(s_1 - c_1)}, \quad z_2 = \frac{(s_2 - c_2 - b)}{(s_2 - c_2)},$$

then we can establish an analogous generating function expansion to (3.78) namely

$$\begin{aligned} Q(z_1, z_2) &= \left(\frac{b}{1 - z_1} \right)^{\alpha_1 + 1} \left(\frac{b}{1 - z_2} \right)^{\alpha_2 + 1} \\ &\quad \times \bar{f} \left(\frac{b}{1 - z_1} + c_1, \frac{b}{1 - z_2} + c_2 \right) \\ &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} Q_{m,n} z_1^m z_2^n, \end{aligned} \quad (3.89)$$

where

$$Q_{m,n} = q_{m,n} \frac{\Gamma(m + \alpha_1 + 1) \Gamma(n + \alpha_2 + 1)}{m! n!}.$$

Moorthy restricts Q to the boundary of the unit polydisc

$$D = \{(z_1, z_2); |z_1| < 1, |z_2| < 1\},$$

by setting

$$\begin{aligned} z_1 &= e^{i\theta_1}, & -\pi &\leq \theta_1 \leq \pi, \\ z_2 &= e^{i\theta_2}, & -\pi &\leq \theta_2 \leq \pi. \end{aligned}$$

On the assumption that f is real it follows that (3.89) can be written as

$$Q(\theta_1, \theta_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} Q_{m,n} e^{i(m\theta_1 + n\theta_2)},$$

from which we deduce that

$$\left. \begin{aligned} Q_{00} &= \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \Re Q(\theta_1, \theta_2) d\theta_1 d\theta_2, \\ Q_{m,n} &= \frac{1}{2\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \Re Q(\theta_1, \theta_2) \cos(m\theta_1 + n\theta_2) d\theta_1 d\theta_2 \end{aligned} \right] . \quad (3.90)$$

Defining Q_1 and Q_2 by

$$\begin{aligned} Q_1(\theta_1, \theta_2) &= \Re[Q(\theta_1, \theta_2)] + \Re[Q(\theta_1, -\theta_2)] \\ Q_2(\theta_1, \theta_2) &= \Re[Q(\theta_1, \theta_2)] - \Re[Q(\theta_1, -\theta_2)] \end{aligned}$$

and applying the midpoint quadrature rule we obtain

$$q_{00} = \frac{1}{2L^2\Gamma(\alpha_1 + 1)\Gamma(\alpha_2 + 1)} \sum_{j=1}^L \sum_{k=1}^L Q_1(\lambda_j, \mu_k), \quad (3.91)$$

and

$$\begin{aligned} q_{m,n} &= \frac{1}{L^2\Gamma(m + \alpha_1 + 1)\Gamma(n + \alpha_2 + 1)} \\ &\times \sum_{j=1}^L \sum_{k=1}^L [Q_1(\lambda_j, \mu_k) \cos(m\lambda_j) \cos(n\mu_k) - Q_2(\lambda_j, \mu_k) \sin(m\lambda_j) \sin(n\mu_k)], \end{aligned} \quad (3.92)$$

where $m, n = 0, 1, \dots, N-1$; $(m, n) \neq (0, 0)$ and

$$\lambda_j = \frac{(2j-1)\pi}{2L}, \quad \mu_k = \frac{(2k-1)\pi}{2L}.$$

Full details about the choice of parameters, the method of summation of the truncated series (3.92) and an error analysis can be found in Moorthy's paper.

Chapter 4

Quadrature Methods

4.1 Interpolation and Gaussian type Formulae

It is not surprising that a number of methods to find the Inverse Laplace transform have, as their basis, the approximation of the Bromwich inversion integral as this provides an explicit solution for $f(t)$ if the integral can be evaluated exactly. Salzer [201] in a series of papers proposed several such methods. He assumes

$$\bar{f}(s) \approx \sum_{r=1}^n \frac{\beta_r}{s^r}, \quad \beta_r \text{ a constant} \quad (4.1)$$

— the absence of the constant term implying that $\bar{f}(s) \rightarrow 0$ as $s \rightarrow \infty$ and, effectively, that $f(t)$ is a polynomial of degree n in t . Salzer evaluates $\bar{f}(s)$ for $s = k$, $k = 1, 2, \dots, n$ and determines the Lagrange interpolation polynomial $p_n(1/s)$ which approximates to $\bar{f}(s)$ at $s = k$, $k = 1, 2, \dots, n$ and $s = \infty$. By this means the β_r are determined which are linear combinations of the $\bar{f}(k)$. Using the known relationship

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{e^s}{s} \left(\frac{1}{s}\right)^r ds = \frac{1}{r!}, \quad (4.2)$$

Salzer determines, for given n , the weights $\alpha_k(t)$ such that

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \bar{f}(s) ds \approx \sum_{k=1}^n \alpha_k(t) \bar{f}(k). \quad (4.3)$$

Additionally, he indicates how one can estimate the error in

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{pt} \left[p_n \left(\frac{1}{s} \right) - \bar{f}(s) \right] ds.$$

The interested reader is referred to Salzer for more details as well as tables of the $\alpha_k(t)$. Shirliffe and Stephenson [209] give a computer adaptation of this

method and report on their experiments to try and find the optimum value of n .

The advantage of using the previous method is that it involves only real calculations. Now that computers are available to ease the burden of computation it is very easy to perform arithmetic involving complex numbers. Salzer notes that if we write $st = u$ we have

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \bar{f}(s) ds = \frac{1}{2\pi i t} \int_{c'-i\infty}^{c'+i\infty} e^u \bar{f}\left(\frac{u}{t}\right) du, \quad (4.4)$$

$\bar{f}(u/t)$ having the same polynomial form in $1/u$ as $\bar{f}(s)$ in $1/s$, that is, not having a constant term, but now involving the parameter t . e^u/u is a weight function for which we can determine orthogonal polynomials $p_n(1/u)$ such that

$$\int_{c'-i\infty}^{c'+i\infty} \frac{e^u}{u} p_n\left(\frac{1}{u}\right) \frac{1}{u^m} du = 0, \quad m = 0, 1, \dots, n-1 \quad (4.5)$$

and hence obtain a Gauss-type quadrature formula which will be accurate for all polynomials of degree $\leq 2n$ in $(1/u)$, whereas the previous method was only accurate for polynomials of degree n . To see how (4.5) arises let $q_{2n}(1/s)$ be any arbitrary $(2n)$ -th degree polynomial in the variable $1/s$ which vanishes at $1/s = 0$. Consider n distinct points $1/s_i$, $i = 1, 2, \dots, n$, other than $1/s = 0$, and construct the $(n+1)$ -point Lagrange interpolation polynomial approximation to $q_{2n}(1/s)$ which is exact at the points $1/s_i$, $i = 1, \dots, n$ and $1/s = 0$. Call this polynomial (which is of degree n) $L^{(n+1)}(1/s)$. Then

$$L^{(n+1)}\left(\frac{1}{s}\right) = \sum_{i=1}^{n+1} L_i^{(n+1)}\left(\frac{1}{s}\right) q_{2n}\left(\frac{1}{s_i}\right), \quad (4.6)$$

where $1/s_{n+1} = 0$ and

$$L_i^{(n+1)}\left(\frac{1}{s}\right) = \prod_{k=1}^{n+1}{}' \left(\frac{1}{s} - \frac{1}{s_k}\right) / \prod_{k=1}^{n+1}{}' \left(\frac{1}{s_i} - \frac{1}{s_k}\right), \quad (4.7)$$

where the prime indicates the absence of $k = i$ in the product. It follows that $q_{2n}(1/s) - L^{(n+1)}(1/s)$ vanishes at $1/s = 0$ and $1/s_i$, $i = 1, 2, \dots, n$ and thus has the factor

$$\frac{1}{s} p_n\left(\frac{1}{s}\right) = \frac{1}{s} \prod_{i=1}^n \left(\frac{1}{s} - \frac{1}{s_i}\right).$$

Writing

$$q_{2n}(1/s) = L^{(n+1)}(1/s) + (1/s) p_n(1/s) r_{n-1}(1/s),$$

where $r_{n-1}(1/s)$ is a polynomial of degree $n-1$ in $1/s$, we have

$$\begin{aligned} \frac{1}{2\pi i} \int_{c'-i\infty}^{c'+i\infty} e^s q_{2n}\left(\frac{1}{s}\right) ds &= \frac{1}{2\pi i} \int_{c'-i\infty}^{c'+i\infty} e^s L^{(n+1)}\left(\frac{1}{s}\right) ds \\ &\quad + \frac{1}{2\pi i} \int_{c'-i\infty}^{c'+i\infty} e^s \frac{1}{s} p_n\left(\frac{1}{s}\right) r_{n-1}\left(\frac{1}{s}\right) ds. \end{aligned} \quad (4.8)$$

Thus if the second term on the right of (4.8) always vanishes, which will be the case when (4.5) holds, then (4.8) will represent an n -point quadrature formula which is exact for any $(2n)$ -th degree polynomial in $1/s$ and yielding the formula

$$\frac{1}{2\pi i} \int_{c'-i\infty}^{c'+i\infty} e^s q_{2n} \left(\frac{1}{s} \right) ds = \sum_{i=1}^n A_i q_{2n} \left(\frac{1}{s_i} \right), \quad (4.9)$$

where the Christoffel numbers are given by

$$A_i = \frac{1}{2\pi i} \int_{c'-i\infty}^{c'+i\infty} e^s L^{(n+1)} \left(\frac{1}{s} \right) ds. \quad (4.10)$$

In order for (4.10) to be computed we need to know the value of the s_i . If we write

$$p_n \left(\frac{1}{s} \right) = \left(\frac{1}{s} \right)^n + b_{n-1} \left(\frac{1}{s} \right)^{n-1} + b_{n-2} \left(\frac{1}{s} \right)^{n-2} + \cdots + b_1 \left(\frac{1}{s} \right) + b_0,$$

and evaluate (4.5) using (4.2) we see that the b_i , $i = 0, \dots, n-1$ satisfy the system of linear equations

$$\begin{aligned} \frac{1}{n!} + \frac{b_{n-1}}{(n-1)!} + \frac{b_{n-2}}{(n-2)!} + \cdots + \frac{b_1}{1!} + \frac{b_0}{0!} &= 0, \\ \frac{1}{(n+1)!} + \frac{b_{n-1}}{n!} + \frac{b_{n-2}}{(n-1)!} + \cdots + \frac{b_1}{2!} + \frac{b_0}{1!} &= 0, \\ \cdot & \quad \cdot \quad \cdot \quad \cdot \quad \cdot \quad \cdot \end{aligned}$$

$$\frac{1}{(2n-1)!} + \frac{b_{n-1}}{(2n-2)!} + \frac{b_{n-2}}{(2n-3)!} + \cdots + \frac{b_1}{n!} + \frac{b_0}{(n-1)!} = 0.$$

We can thus determine the roots of the polynomial equation $p_n(1/s) = 0$ by using a polynomial solver (or alternatively find the eigenvalues of the companion matrix - see Appendix 11.7). An alternative procedure is to use the fact that orthogonal polynomials satisfy 3-term recurrence relationships and associate this with a tridiagonal matrix (see Cohen [45]) whose eigenvalues can be determined using a standard technique such as the QR method.

Salzer shows that if we write

$$\begin{aligned} P_1(x) &= p_1(x) \quad (= x-1); \quad P_2(x) = 6x^2 - 4x + 1 \\ P_n(x) &= (4n-2)(4n-6) \cdots 6p_n(x), \quad n \geq 2 \end{aligned}$$

then $P_n(x)$ satisfies the recurrence relation

$$P_{n+1}(x) = \left[(4n+2)x + \frac{2}{2n-1} \right] P_n(x) + \frac{2n+1}{2n-1} P_{n-1}(x), \quad n \geq 2. \quad (4.11)$$

Clearly, the roots of $P_n(x)$ and $p_n(x)$ are identical and if they are x_1, \dots, x_n then $s_i = 1/x_i$, $i = 1, \dots, n$.

Another way of looking at the problem of generating the abscissae and weights in the Gaussian n -point quadrature formula

$$\frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \bar{f}(s) ds \approx \sum_{k=1}^n \alpha_k(t) \bar{f}(s_k), \quad (4.12)$$

has been provided by Zakian [262], [263]. He shows that the polynomial $p_n(x)$ is the denominator in the $[n-1/n]$ Padé approximant (see §11.5) to the function $e^{1/x}$. Thus when $n = 2$, the polynomial $P_2(x) = 6x^2 - 4x + 1$, given previously, is the $[1/2]$ Padé approximant. The weights are related to the residues of the $[n-1/n]$ Padé approximant.

Piessens [169], [172] extended this idea to the case where

$$s^\nu \bar{f}(s) \simeq \sum_0^{n-1} \frac{\beta_r}{s^r}, \quad \nu > 0, \quad (4.13)$$

and obtained Gaussian n -point formulae for $\bar{f}(s)$ having this behaviour. He showed that the abscissae and weights of the Gauss quadrature formula, when $\bar{f}(s)$ is defined by (4.13), are connected with the $[n-1/n]$ Padé approximants of the power series

$$\sum_{k=0}^{\infty} \frac{1}{x^k \Gamma(\nu + k)}. \quad (4.14)$$

Moreover, he showed that the real parts of the abscissae are all positive. For a detailed summary of these developments see [216], pp 439 et seq. where an additional quadrature method derived from the Sidi \mathcal{S} -transformation applied to the series (4.14) can be found.

It is important to know the exact value of ν to obtain satisfactory results. For example with

$$\bar{f}(s) = (s^2 + 1)^{-1/2},$$

$\nu = 1$ and thus we have exactly the Salzer case. A 12-point formula in this case gives results with almost 10 decimal place accuracy for $1 \leq t \leq 8$ but only 3 decimal place accuracy is achieved for $t = 16$. For

$$\bar{f}(s) = s^{-1/2} \exp(-s^{-1/2}),$$

we require $\nu = 1/2$ and results of almost 12 decimal place accuracy were obtained for $1 \leq t \leq 100$. But the case $\bar{f}(s) = s \ln s / (s^2 + 1)$ does not fit into the pattern (4.13) and Piessens had to give a special treatment for this type of logarithmic behaviour.

4.2 Evaluation of Trigonometric Integrals

Schmittroth [206] described a numerical method for inverting Laplace transforms which is based on a procedure of Hurwitz and Zweifel [113] for evaluating trigonometric integrals. Schmittroth assumes that all singularities of $f(s)$ lie in $\Im s < 0$, and hence we can take $c = 0$ in the inversion formula, i.e.

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{f}(i\omega) e^{i\omega t} d\omega, \quad t > 0. \quad (4.15)$$

If we write $\phi(\omega) = \Re \bar{f}(i\omega)$ and $\psi(\omega) = -\Im \bar{f}(i\omega)$ then, as we can assume that $f(\bar{s}) = \overline{f(s)}$, where the bar denotes complex conjugation, it follows that $\phi(\omega)$ is an even function and $\psi(\omega)$ is an odd function. Moreover, we can deduce from Chapter 2 that

$$f(t) = \frac{2}{\pi} \int_0^{\infty} \phi(\omega) \cos t\omega d\omega, \quad (4.16)$$

or

$$f(t) = \frac{2}{\pi} \int_0^{\infty} \psi(\omega) \sin t\omega d\omega. \quad (4.17)$$

To evaluate the above integrals Hurwitz and Zweifel made the transformation $y = \omega t/\pi$ in (4.16) and $u = (\omega t/\pi) - \frac{1}{2}$ in (4.17). For the derivation of the method they extend the definition of the functions ϕ and ψ to negative values of ω by requiring ϕ to be even and ψ to be odd. (This is unnecessary in our case because of the way the functions have been derived). If we just concentrate on the sine integral (4.17) we see that it can be written as

$$f(t) = \frac{1}{t} \int_{-1/2}^{1/2} \cos \pi u g(u, t) du, \quad (4.18)$$

where

$$g(u, t) = \sum_{n=-\infty}^{\infty} (-1)^n \psi \left(\frac{\pi}{t} \left[u + n + \frac{1}{2} \right] \right). \quad (4.19)$$

The function $g(u, t)$ has the following properties

- (a) $g(u, t) = g(-u, t)$,
- (b) $g(\frac{1}{2}, t) = g(-\frac{1}{2}, t) = 0$,
- (c) $g(u + n, t) = (-1)^n g(u, t)$,
- (d) g is regular, $-\frac{1}{2} \leq u \leq \frac{1}{2}$ if $\psi(\omega)$ is regular for $-\infty < \omega < \infty$.

Because of these properties g can be expanded as a Fourier series of the form

$$g(u, t) = \sum_{n=0}^{\infty} a_n(t) \cos(2n+1)\pi u, \quad (4.20)$$

and, since $\cos n\theta$ is a polynomial of degree n in $\cos \theta$, we have

$$g(u, t) = \cos \pi u \sum_{n=0}^{\infty} \alpha_n(t) \cos^{2n} \pi u. \quad (4.21)$$

If we treat the cosine integral (4.16) similarly we arrive at a function $h(y, t)$ which has a similar expansion to the function g in (4.21).

Substitution of (4.21) in (4.18) gives

$$f(t) = \frac{1}{t} \int_{-1/2}^{1/2} \cos^2 \pi u \sum_{n=0}^{\infty} \alpha_n(t) \cos^{2n} \pi u, \quad (4.22)$$

The function $w(u) = \cos^2 \pi u$ occurring in the integrand is clearly a positive weight function and Hurwitz and Zweifel establish a Gaussian quadrature formula by first determining the set of polynomials $p_n(\cos \pi u)$ which are orthogonal with respect to the weight function $w(u)$ over the interval $[-\frac{1}{2}, \frac{1}{2}]$. It turns out that

$$\begin{aligned} p_n(\cos \pi u) &= T_{2n+1}(\cos \pi u) / \cos \pi u, \\ &= \cos(2n+1)\pi u / \cos \pi u, \end{aligned} \quad (4.23)$$

where the polynomial $T_n(x)$ is the Chebyshev polynomial of the first kind of degree n . The $2N$ -point Gaussian quadrature formula is

$$\int_{-1/2}^{1/2} \cos \pi u g(u, t) du = \sum_{j=1}^N \frac{2W_j^{(N)}}{\cos \pi u_j^{(N)}} g(u_j^{(N)}, t), \quad (4.24)$$

where the $u_j^{(N)}$ are the zeros of $p_N(\cos \pi u) = 0$, i.e.,

$$u_j^{(N)} = \frac{2j-1}{2(2N+1)}, \quad j = 1, 2, \dots, N, \quad (4.25)$$

and the W_j are the Christoffel numbers. These may be determined from equation (11.25) in Appendix 11.3 or by solution of the N simultaneous equations

$$\sum_{j=1}^N \cos^{2k-2} \left(\frac{(2j-1)\pi}{2(2N+1)} \right) W_j^{(N)} = \frac{1}{2\sqrt{\pi}} \frac{\Gamma(k + \frac{1}{2})}{\Gamma(k+1)}, \quad k = 1, 2, \dots, N. \quad (4.26)$$

Then $f(t)$ can be computed from

$$f(t) = \frac{2e^{ct}}{t} \sum_{n=0}^{\infty} I_n(t), \quad (4.27)$$

where

$$I_n(t) = (-1)^n \int_{-1/2}^{1/2} \psi \left(\frac{\pi}{t} \left[u + n + \frac{1}{2} \right] \right). \quad (4.28)$$

$I_n(t)$ is computed using the N -point formula of Hurwitz and Zweifel. If $S_m^{(0)}$ denotes $\sum_{n=0}^m I_n$ then Schmittroth used Hutton's averaging procedure (§11.4)

$$S_m^{(k)} = (S_m^{(k-1)} + S_{m+1}^{(k-1)})/2, \quad k = 1, 2, \dots \quad (4.29)$$

to speed up convergence. While this procedure has some merit a better approach would be to use some other extrapolation technique after ensuring that N is chosen sufficiently large to obtain accurate results. It is worth noting that the method becomes increasingly accurate for fixed N as t increases and thus is more reliable for $t > t_{\min}$, for some value t_{\min} dependent on N , while other methods such as FFT are more reliable for $t < t_{\max}$.

4.3 Extrapolation Methods

If we make the substitution $s = c + ix$ in the Bromwich integral we have

$$f(t) = \frac{e^{ct}}{2\pi} \int_{-\infty}^{\infty} e^{ixt} \bar{f}(c + ix) dx. \quad (4.30)$$

One approach to evaluating infinite integrals of this kind is by convergence acceleration. Methods which have enjoyed some success are the confluent ϵ -algorithm of Wynn [257] and the G-transformation of Gray, Atchison and McWilliams [105]. In their original form there were some computational difficulties associated with these methods as the former requires computation of high order derivatives and the latter computation of high order determinants. However, it has now been shown that the G-transformation can be implemented efficiently (without computing high order determinants) by the rs-algorithm of Pye and Atchison [191] or through the FS/qd-algorithm of Sidi [216], the latter being the more efficient of the two. Despite this improvement in computing the G-transformation it is more (computationally) expensive than the Levin P-transformation and the Sidi mW-transformation.

4.3.1 The P -transformation of Levin

The Levin P-transformation [127] has a similar derivation to the Levin t -transformation for series. (4.30) can be written in the form

$$f(t) = \frac{e^{ct}}{2\pi} \left[\int_{-\infty}^0 + \int_0^{\infty} \right] e^{ixt} \bar{f}(c + ix) dx, \quad (4.31)$$

which leads to consideration of a Fourier integral of the form $\int_0^{\infty} g(x) e^{i\omega x} dx$. If

$$x^{\nu} g(x) = \sum_{k=0}^{\infty} \frac{\beta_k}{x^k}, \quad \nu > 0,$$

then Levin showed that one can obtain an asymptotic expansion for $\int_u^\infty g(x)e^{i\omega x} dx$ of the form

$$\int_u^\infty g(x)e^{i\omega x} dx \sim b(u)e^{i\omega u} \sum_{k=0}^\infty \frac{\gamma_k}{u^k}.$$

On the above assumption if we call $A = \int_0^\infty g(x)e^{i\omega x} dx$ and let $A(u) = \int_0^u g(x)e^{i\omega x} dx$ be its finite part then truncation of the asymptotic expansion at the term u^{-k} gives

$$A - A(u) \equiv \int_u^\infty g(x)e^{i\omega x} dx \approx b(u)e^{i\omega u} \sum_{j=0}^{k-1} \frac{\gamma_j}{u^j}. \quad (4.32)$$

Levin demanded that the approximation P to A obeyed the relationship (4.32) exactly for $k+1$ equidistant values of u , i.e.,

$$P - A(u + n\Delta u) = b(u + n\Delta u)e^{i\omega(u+n\Delta u)} \sum_{j=0}^{k-1} \frac{\gamma_j}{(u + n\Delta u)^j}, \quad n = 0, 1, \dots, k \quad (4.33)$$

This gives $k+1$ linear equations in the $k+1$ unknowns $P, \gamma_0, \gamma_1, \dots, \gamma_{k-1}$ which are similar to the equations defining the t -transformation (see Appendix 11.4). If we relate this to the Bromwich integral (4.31) Levin obtained the approximation P_k to $f(t)$ given by

$$P_k = \frac{e^{ct}}{\pi} \Re \left(\frac{\sum_{j=0}^k (-1)^j \binom{k}{j} (j+1)^{k-1} \left[\frac{I_{j+1}(t)e^{-i(j+1)t}}{\bar{f}(c+i(j+1))} \right]}{\sum_{j=0}^k (-1)^j \binom{k}{j} (j+1)^{k-1} \left[\frac{e^{-i(j+1)t}}{\bar{f}(c+i(j+1))} \right]} \right) \quad (4.34)$$

where $I_{j+1}(t) = A(j+1) = \int_0^{j+1} e^{ixt} \bar{f}(c+ix) dx$. In practice these quantities $I_{j+1}(t)$ must be evaluated by some quadrature formula and Levin used a Gauss-Legendre quadrature formula which was of sufficiently high order to ensure 14 correct significant digits for the integral.

4.3.2 The Sidi mW-Transformation for the Bromwich integral

The Sidi mW-transformation described in [216], Chapter 11 can be summarized as follows:

Sidi writes the Bromwich integral in the form

$$f(t) = \frac{e^{ct}}{2\pi} \left[\int_0^\infty e^{i\omega t} \bar{f}(c+i\omega) d\omega + \int_0^\infty e^{-i\omega t} \bar{f}(c-i\omega) d\omega \right] \quad (4.35)$$

$$= \frac{e^{ct}}{2\pi} [u_+(t) + u_-(t)], \quad (4.36)$$

where

$$u_{\pm}(t) = \int_0^{\infty} e^{\pm i\omega t} \bar{f}(c \pm i\omega) d\omega, \quad (4.37)$$

and approximates the integrals $u_{\pm}(t)$ by the mW-transformation. When the Laplace transform of $f(t)$ can be expressed in the form

$$\bar{f}(s) = \exp(-st_0)g(s),$$

where $g(s)$ has an asymptotic expansion of the form

$$g(s) \sim \sum_{i=0}^{\infty} \alpha_i s^{\delta-i} \quad \text{as } s \rightarrow \infty.$$

Sidi then takes the following steps:-

1. Set

$$\omega_{\ell} = (\ell + 1)\pi/(t - t_0), \quad \ell = 0, 1, \dots \quad (4.38)$$

2. Compute the integrals

$$\psi_{\pm}(\omega_{\ell}) = \int_{\omega_{\ell}}^{\omega_{\ell+1}} e^{\pm i\omega t} \bar{f}(c \pm i\omega) d\omega, \quad \ell = 0, 1, \dots, \quad (4.39)$$

and

$$V_{\pm}(\omega_{\ell}) = \int_0^{\omega_{\ell}} e^{\pm i\omega t} \bar{f}(c \pm i\omega) d\omega = \sum_{k=0}^{\ell-1} \psi_{\pm}(\omega_k), \quad \ell = 0, 1, \dots \quad (4.40)$$

3. Solve the linear system of equations

$$V_{\pm}(\omega_{\ell}) = W_n^{(\pm, j)} + \psi_{\pm}(\omega_{\ell}) \sum_{i=0}^{n-1} \frac{\beta_i}{\omega_{\ell}}, \quad \ell = j, j+1, \dots, j+n, \quad (4.41)$$

in order to determine $W_n^{(\pm, j)}$ as $W_n^{(\pm, j)} \approx u_{\pm}(t)$ — the unknowns β_i , $i = 0, 1, \dots, n-1$ are not of interest.

The solution for $W_n^{(\pm, j)}$ can be achieved in an efficient manner via the W-algorithm of Sidi which follows. For convenience of notation the symbol \pm has been suppressed.

- 1' For $j = 0, 1, \dots$ set

$$M_0^{(j)} = \frac{V(\omega_j)}{\psi(\omega_j)}, \quad N_j^{(j)} = \frac{1}{\psi(\omega_j)}. \quad (4.42)$$

2' For $j = 0, 1, \dots$ and $n = 1, 2, \dots$ compute

$$M_n^{(j)} = \frac{M_{n-1}^{(j+1)} - M_{n-1}^{(j)}}{\omega_{j+n}^{-1} - \omega_j^{-1}}, \quad N_n^{(j)} = \frac{N_{n-1}^{(j+1)} - N_{n-1}^{(j)}}{\omega_{j+n}^{-1} - \omega_j^{-1}}. \quad (4.43)$$

3' For all j and n set

$$W_n^{(j)} = \frac{M_n^{(j)}}{N_n^{(j)}}. \quad (4.44)$$

The quantities $W_n^{(\pm, j)}$ converge to $u_{\pm}(t)$ very quickly as $n \rightarrow \infty$ with j fixed ($j = 0$, for example). In fact,

$$W_n^{(\pm, j)} - u_{\pm}(t) = O(n^{-\mu}) \quad \text{as } n \rightarrow \infty, \text{ for any } \mu > 0. \quad (4.45)$$

Thus, it is sufficient to take $W_n^{(\pm, 0)}$, $n = 1, 2, \dots$ as the approximation to $u_{\pm}(t)$.

In the case where $f(t)$ is a real function we have $u_{-}(t) = \overline{u_{+}(t)}$ hence

$$f(t) = \frac{e^{ct}}{\pi} \Re \left[\int_0^{\infty} e^{i\omega t} \bar{f}(c + i\omega) d\omega \right], \quad (4.46)$$

and we need only compute one of $u_{\pm}(t)$.

The key to the success of the mW-transformation is the correct choice of the ω_{ℓ} . These are chosen so that $\text{sign}[\phi(\omega_{\ell})\phi(\omega_{\ell+1})] = -1$ for all large ℓ , where $\phi(\omega) = e^{i\omega t} \bar{f}(c + i\omega)$. Surprisingly, the method we have described above may still work even when the function $\bar{f}(s)$ is not precisely as described above, but $\text{sign}[\phi(\omega_{\ell})\phi(\omega_{\ell+1})] = -1$ for all large ℓ . For example, very good approximations are obtained for the test function f_{35} in Section 9.4.

In some cases, where $\bar{f}(s)$ does not behave the way we described above, it may still be possible to choose the ω_{ℓ} to guarantee that $\text{sign}[\phi(\omega_{\ell})\phi(\omega_{\ell+1})] = -1$ for all large ℓ , and this is the most general case described in Sidi [214]. Let us consider the test function $f_{15}(t)$ in Section 9.4, for example. We have, since $\bar{f}_{15}(s) = e^{-4s^{1/2}}$,

$$\begin{aligned} \phi(\omega) &= e^{i\omega t} e^{-4(c+i\omega)^{1/2}}, \\ &= e^{i[\omega t + 4i(c+i\omega)^{1/2}]} = e^{i\eta(\omega)}. \end{aligned}$$

Expansion of $\eta(\omega)$ gives

$$\eta(\omega) = \omega t + 4ie^{i\pi/4}\omega^{1/2} + O(\omega^{-1/2}) \quad \text{as } \omega \rightarrow \infty.$$

This implies

$$\Re\eta(\omega) = \omega t - 2^{3/2}\omega^{1/2} + O(\omega^{-1/2}) \quad \text{as } \omega \rightarrow \infty.$$

Thus the appropriate choice for the ω_{ℓ} are the positive zeros of

$$\sin(\omega t - 2^{3/2}\omega^{1/2}) = 0,$$

that is

$$\omega_\ell = \left\lceil \frac{\sqrt{2} + \sqrt{2 + (\ell + 1)\pi t}}{t} \right\rceil^2, \ell = 0, 1, \dots. \quad (4.47)$$

It is important to make sure that the integrals $\psi(\omega_\ell)$ in (4.39) are computed accurately. The computation may be expensive when the singularities of $\bar{f}(s)$ are close to the interval $I_\ell = [c + ix_\ell, c + ix_{\ell+1}]$ in the sense that the ratio

$$\frac{\text{distance of a point of singularity of } \bar{f}(s) \text{ to } I_\ell}{\text{length of interval } I_\ell}, \quad (I_\ell = \omega_{\ell+1} - \omega_\ell)$$

is small. This is the case when t is small so that in this case c could be increased somewhat. This is a very effective method for evaluating the inverse transform. Because of the equivalence of (4.46) with A and B where

$$A = \frac{2e^{ct}}{\pi} \int_0^\infty \Re[f(c + i\omega)] \cos \omega t d\omega \quad (4.48)$$

and

$$B = -\frac{2e^{ct}}{\pi} \int_0^\infty \Im[f(c + i\omega)] \sin \omega t d\omega \quad (4.49)$$

this author has computed A and B in preference to (4.46) as the agreement in decimal places gives a practical indication of the likely accuracy of the result. A program is provided at the website

www.cf.ac.uk/maths/cohen/programs/inverselaplace transform/.

This approach seems to work well when $\bar{f}(s)$ belongs to the class of functions outlined above and will give good results for the functions $f_1(t)$, $f_3(t)$, $f_{25}(t)$, $f_{30}(t)$ — see the survey in Chapter 9. Prior numerical experience shows that it will also work for $f_{11}(t)$ and $f_{35}(t)$. In the case of $f_{15}(t)$ the choice of $\omega_\ell = (\ell + 1)\pi/t$ gives poor results and we would need to choose ω_ℓ satisfying (4.47) to get good approximations to $f_{15}(t)$.

4.4 Methods using the Fast Fourier Transform (FFT)

The methods of the previous two sections involved the evaluation of a Fourier integral. Dubner and Abate [71] developed a method for inverting the Laplace transform by relating the Fourier integral to a finite Fourier cosine transform. Given a real function $h(t)$ for which $h(t) = 0$ for $t < 0$ they constructed a set of even periodic functions $g_n(t)$ of period $2T$ such that for $n = 0, 1, 2, \dots$ we have

$$g_n(t) = \begin{cases} h(t), & nT \leq t \leq (n+1)T, \\ h(2nT - t), & (n-1)T \leq t \leq nT. \end{cases} \quad (4.50)$$

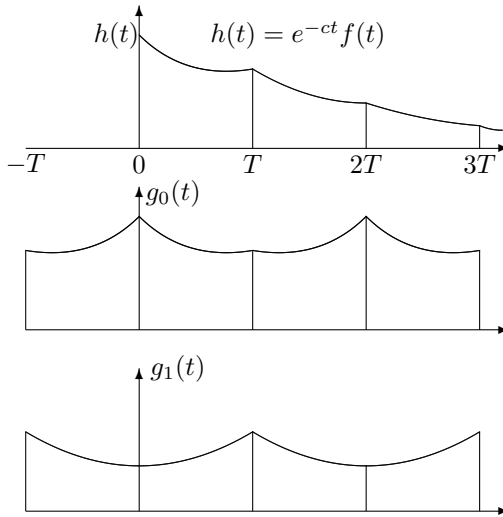


Figure 4.1: Function representation by even Fourier series

This is equivalent to defining $g_n(t)$ in $(-T, T)$ by

$$g_n(t) = \begin{cases} h(nT + t), & 0 \leq t \leq T, \\ h(nT - t), & -T \leq t \leq 0, \end{cases} \quad (4.51)$$

for $n = 0, 2, 4, \dots$ and

$$g_n(t) = \begin{cases} h((n+1)T - t), & 0 \leq t \leq T, \\ h((n+1)T + t), & -T \leq t \leq 0. \end{cases} \quad (4.52)$$

for $n = 1, 3, 5, \dots$ (see fig. 4.1).

The Fourier cosine representation of each $g_n(t)$ is given for all n by

$$g_n(t) = \frac{1}{2}A_{n,0} + \sum_{k=1}^{\infty} A_{n,k} \cos\left(\frac{k\pi t}{T}\right), \quad (4.53)$$

where the coefficients, which are finite cosine transforms, can be expressed as

$$A_{n,k} = \frac{2}{T} \int_{nT}^{(n+1)T} h(t) \cos\left(\frac{k\pi t}{T}\right) dt. \quad (4.54)$$

If we sum (4.53) over n we get

$$\sum_{n=0}^{\infty} g_n(t) = \frac{2}{T} \left[\frac{1}{2}A(\omega_0) + \sum_{k=1}^{\infty} A(\omega_k) \cos\left(\frac{k\pi t}{T}\right) \right], \quad (4.55)$$

where

$$A(\omega_k) = \int_0^\infty h(t) \cos\left(\frac{k\pi t}{T}\right) dt. \quad (4.56)$$

Dubner and Abate note that $A(\omega_k)$ is a Fourier cosine transform and by letting

$$h(t) = e^{-ct} f(t), \quad (4.57)$$

it is seen to be the Laplace transform of a real function $f(t)$ with the transform variable being given by $s = c + i(k\pi/T)$. That is, $A(\omega_k) = \Re \bar{f}(s)$. Thus (4.55) becomes

$$\sum_{n=0}^{\infty} e^{ct} g_n(t) = \frac{2e^{ct}}{T} \left[\frac{1}{2} \Re \bar{f}(c) + \sum_{k=1}^{\infty} \Re \left\{ \bar{f} \left(c + \frac{k\pi i}{T} \right) \right\} \cos \frac{k\pi t}{T} \right]. \quad (4.58)$$

The left hand side of (4.58) is almost the inverse Laplace transform of $\bar{f}(s)$ in the interval $(0, T)$, but it contains an error. From (4.51) and (4.52) we have

$$\sum_{n=0}^{\infty} e^{ct} g_n(t) = \sum_{n=0}^{\infty} e^{ct} h(2nT + t) + \sum_{n=0}^{\infty} e^{ct} h(2nT - t).$$

The first term on the right hand side is $f(t)$ and thus

$$\sum_{n=0}^{\infty} e^{ct} g_n(t) = f(t) + E_1, \quad (4.59)$$

where the error E_1 is given by

$$E_1 = \sum_{n=1}^{\infty} \exp(-2cTn) [f(2nT + t) + \exp(2ct) f(2nT - t)]. \quad (4.60)$$

Dubner and Abate show that E_1 can only be made small for $t \leq T/2$ and they conclude that for the interval $(0, T/2)$ the inverse Laplace transform can be found to any desired accuracy by the formula

$$f(t) \simeq \frac{2e^{ct}}{T} \left[\frac{1}{2} \Re \bar{f}(c) + \sum_{k=1}^{\infty} \Re \left\{ \bar{f} \left(c + \frac{k\pi i}{T} \right) \right\} \cos \frac{k\pi t}{T} \right], \quad (4.61)$$

where on the right hand side we are evaluating the Laplace transform. Dubner and Abate show that Fast Fourier Transform (FFT) methods can be employed to reduce computation in (4.61) if $f(t)$ is required for a significant number of t values. If $f(t)$ is required at the equidistant points $t = j\Delta t$ where $j = 0, 1, 2, \dots, \frac{1}{4}N$, i.e. $t_{\max} = \frac{1}{4}N\Delta t$ then we can compute $f(t)$ in the following way:- We compute

$$A(k) = \frac{1}{N\Delta t} \sum_{n=-\infty}^{\infty} \Re \left\{ \bar{f} \left(c + \frac{2\pi i}{N} (k + nN) \right) \right\}, \quad k = 0, 1, \dots, N-1 \quad (4.62)$$

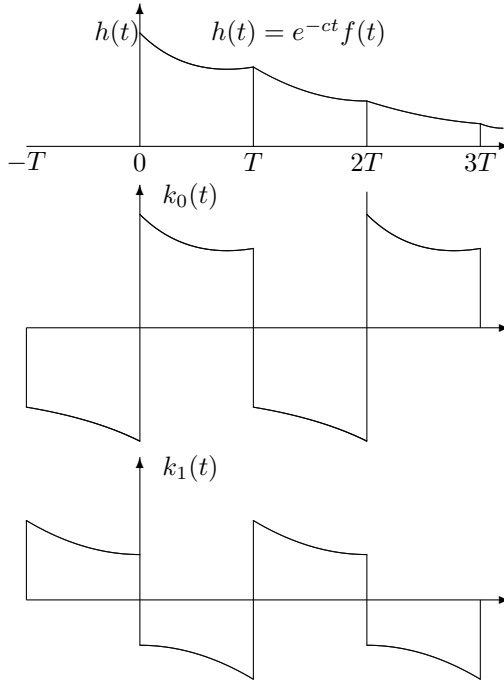


Figure 4.2: Function representation by odd Fourier series

then use the FFT routine to determine $f(j\Delta t)/b(j)$ from

$$\frac{f(j\Delta t)}{b(j)} = \sum_{k=0}^{N-1} A(k) \exp\left(\frac{2\pi i}{N} jk\right), \quad (4.63)$$

where $b(j) = 2 \exp(aj\Delta t)$. The value of $f(j\Delta t)$ is accepted as a representation of the function f for $j \leq \frac{1}{4}N$.

Durbin [73] showed that an alternative procedure to that of Dubner and Abate could be obtained if we constructed a set of odd periodic functions $k_n(t)$, say, with the property that, for each $n > 0$

$$k_n(t) = \begin{cases} h(t) & nT \leq t \leq (n+1)T \\ -h(2nT - t) & (n-1)T \leq t \leq nT \end{cases} \quad (4.64)$$

(see fig. 4.2).

Proceeding as before we have the Fourier representation for each $k_n(t)$ is

$$k_n(t) = \sum_{k=0}^{\infty} B_{n,k} \sin\left(\frac{k\pi t}{T}\right), \quad (4.65)$$

where

$$B_{n,k} = \int_{nT}^{(n+1)T} e^{-ct} f(t) \sin\left(\frac{k\pi t}{T}\right) dt. \quad (4.66)$$

This leads to

$$\sum_{n=0}^{\infty} e^{ct} k_n(t) = -\frac{2e^{ct}}{T} \left[\Im \left\{ \bar{f} \left(c + \frac{ik\pi}{T} \right) \right\} \sin\left(\frac{k\pi t}{T}\right) \right].$$

But we also have

$$\sum_{n=0}^{\infty} e^{ct} k_n(t) = f(t) + \sum_{k=1}^{\infty} e^{-2ckT} [f(2kT + t) - e^{2ct} f(2kT - t)],$$

and hence

$$f(t) + E_2 = -\frac{2e^{ct}}{T} \left[\Im \left\{ \bar{f} \left(c + \frac{ik\pi}{T} \right) \right\} \sin\left(\frac{k\pi t}{T}\right) \right], \quad (4.67)$$

where E_2 is given by

$$E_2 = \sum_{k=1}^{\infty} e^{-2ckT} [f(2kT + t) - e^{2ct} f(2kT - t)]. \quad (4.68)$$

Durbin points out that this approach yields essentially the same result as the method of Dubner and Abate but now the error term has the opposite sign. Consequently the error bound can be reduced considerably by averaging (4.58) and (4.67). We have now

$$\begin{aligned} f(t) + E_3 = \frac{e^{ct}}{T} & \left[\frac{1}{2} \Re\{\bar{f}(c)\} + \sum_{k=1}^{\infty} \Re \left\{ \bar{f} \left(c + \frac{ik\pi}{T} \right) \right\} \cos\left(\frac{k\pi t}{T}\right) \right. \\ & \left. - \sum_{k=1}^{\infty} \Im \left\{ \bar{f} \left(c + \frac{ik\pi}{T} \right) \right\} \sin\left(\frac{k\pi t}{T}\right) \right], \end{aligned} \quad (4.69)$$

where

$$E_3 = \sum_{k=1}^{\infty} e^{-2ckT} f(2kT + t). \quad (4.70)$$

Since $\bar{f}(s)$ may be assumed to have no singularities for $\Re s > 0$ it follows that $f(t)$ is bounded at infinity by some function of the form κt^m where κ is a constant and m is a non-negative integer. If $|f(t)| < \kappa$ then

$$|E_3| < \sum_{k=1}^{\infty} \kappa e^{-2kcT} = \frac{\kappa}{e^{2cT} - 1} \quad (4.71)$$

In the more general case we have

$$\begin{aligned}
 |E_3| &< \sum_{k=1}^{\infty} e^{-2kcT} \kappa(t + 2kT)^m \\
 &< \kappa(2T)^m \sum_{k=1}^{\infty} e^{-2kcT} (k+1)^m \\
 &< \kappa(2T)^m \int_1^{\infty} e^{-2xcT} (x+1)^m dx
 \end{aligned}$$

The integral may be computed by integration by parts and we obtain

$$|E_3| < K(2T)^m e^{-2cT} \sum_{i=1}^{m+1} \frac{\alpha_i}{(2cT)^i} \quad (4.72)$$

where $K, \alpha_1, \dots, \alpha_{m+1}$ are constants. Clearly the error term decreases rapidly with cT but it also depends on T . Durbin notes that the approximation given by (4.69) is equivalent to applying a trapezoidal rule with step π/T but his strategy has resulted in an error bound proportional to $\exp(-2cT)$ whereas, in general, the error bound is $O(1/T^2)$. Finally, he uses the Fast Fourier Transform to implement the inversion.

Despite the apparent smallness of the error bound in Fourier series methods we note that, following Sidi [215], because the Fourier series is multiplied by a factor e^{ct} , this could result in the theoretical error being dominated by the computational error. More precisely, denoting the term in square brackets in (4.69) by $S(t)$, we have

$$\left| f(t) - \frac{e^{ct}}{T} S(t) \right| = |E_3| < C(T) e^{-2cT}, \quad t \in (0, 2T),$$

where $C(T)$ is a constant which depends on T . If we make an error ϵ in computing $S(t)$, that is, we compute $S_1(t)$ where $S_1(t) = S(t) + \epsilon$ then the error in computing $f(t)$ is given by

$$\begin{aligned}
 \left| f(t) - \frac{e^{ct}}{T} S_1(t) \right| &\leq \left| f(t) - \frac{e^{ct}}{T} S(t) \right| + \frac{e^{ct}}{T} |S(t) - S_1(t)|, \\
 &\leq C(T) e^{c(t-2T)} / T + \epsilon e^{ct} / T.
 \end{aligned}$$

It follows that if ϵ is too large the computational error may dominate the theoretical error. This is particularly the case for t large and close to $2T$.

Crump [53] uses the formula (4.69) in a different way. By assuming that $|f(t)| \leq M e^{\gamma t}$ he finds that

$$E_3 \leq M e^{\gamma t} / (e^{2T(c-\gamma)} - 1), \quad 0 < t < 2T. \quad (4.73)$$

Thus by choosing c sufficiently larger than γ we can make E_3 as small as desired. For convergence to at least 2 significant figures, say, this means that we require

the relative error $E_R \equiv E_3/Me^{\gamma t} \leq 0.005$, so that for all practical purposes (4.73) can be replaced by

$$E_3 \leq Me^{\gamma t} e^{-2T(c-\gamma)}, \quad 0 < t < 2T. \quad (4.74)$$

Crump points out that the case $t = 0$ has to be analysed separately since there will usually be a discontinuity at $t = 0$ in the Fourier series representation for $f(t)e^{-ct}$, call it $g^*(t)$, in $0 \leq t < 2T$. In fact $g^*(0) = [f(0) + e^{-2cT}f(2T)]/2$. Thus at $t = 0$ the method approximates $\frac{1}{2}f(0)$ with error $E_3 + f(2T)\exp(-2cT)/2 \approx \frac{3}{2}E_3$ which is approximately 50 percent greater than the error bound for $t > 0$.

The error bound (4.74) provides a simple algorithm for computing $f(t)$ to prescribed accuracy. If we require the numerical value of $f(t)$ over a range of t for which the largest is t_{\max} and the relative error is to be smaller than E' then we choose T such that $2T > t_{\max}$ and use (4.74) to compute c , i.e. we choose

$$c = \gamma - (\ln E')/2T. \quad (4.75)$$

γ can be computed from the transform $\bar{f}(s)$ by determining the pole which has largest real part. The series on the right hand side in (4.69) is then summed until it has converged to the desired number of significant figures. However convergence may be slow and Crump uses the epsilon algorithm (see §11.4) to speed the convergence. The reader can download a sample program using NAG Library Routine C06LAF which is based on Crump's method at the URL www.cf.ac.uk/maths/cohen/programs/inverselaplace/transform/. The idea of speeding up convergence had previously been considered by Simon, Stroot and Weiss [219] who had used Euler's method of summation (see §11.4). This approach was effective but superior results were achieved by Crump's method. Veillon [243] also applies the epsilon algorithm but uses it with the Dubner and Abate summation (4.61). A novel feature of her method is the use of splines to estimate the "best" value of c .

De Hoog et al [64] point out that the coefficients in the Fourier series are derived from an infinite sum and the formal manipulation used to derive them is only valid if we have uniform convergence. This would not be the case for example if $\bar{f}(s) = 1/s$ and we are using the Durbin/Crump approach. They also find some drawbacks in using the epsilon algorithm as round-off error can make the process numerically unstable if a large number of diagonals are employed. De Hoog et al opt to retain the original complex form to determine the inverse Laplace transform. That is they aim to compute

$$g(t) = \frac{1}{2}\bar{f}(\gamma) + \sum_{k=1}^{\infty} \bar{f}\left(\gamma + \frac{ik\pi}{T}\right) \exp\left(\frac{ik\pi t}{T}\right) = \sum_{k=0}^{\infty} a_k z^k, \quad (4.76)$$

with $a_0 = \frac{1}{2}\bar{f}(\gamma)$, $a_k = \bar{f}(\gamma + ik\pi/T)$, $k = 1, 2, \dots$ and $z = \exp(i\pi t/T)$. Instead of applying the epsilon algorithm to the partial sums of (4.76), which involves calculating the epsilon table for each particular value of z , they use the quotient-difference algorithm which makes the rational approximation available

in the form of a continued fraction (see §11.5). This enables the series (4.76) to be evaluated at any time value by recursion. Given the power series (4.76) we want to calculate the continued fraction

$$v(z) = \frac{d_0}{1+} \frac{d_1 z}{1+} \frac{d_2 z}{1+ \dots},$$

which has the same power series development. In practice this means determining $v_{2M}(z)$ where

$$u_{2M}(z) = \sum_{k=0}^{2M} a_k z^k, \quad v_{2M}(z) = \frac{d_0}{1+} \frac{d_1 z}{1+ \dots} \frac{d_{2M} z}{1},$$

and

$$u_{2M}(z) - v_{2M}(z) = O(z^{2M+1}),$$

i.e. $v_{2M}(z)$ is the same diagonal Padé approximant as $\varepsilon_{2M}^{(0)}$. The coefficients d_k can be calculated using the quotient-difference algorithm as follows. We set $e_0^{(i)} = 0$ for $i = 0, \dots, 2M$ and $q_1^{(i)} = a_{i+1}/a_i$ for $i = 0, \dots, 2M - 1$. Successive columns of the array are then determined from

$$e_r^{(i)} = q_r^{(1+i)} - q_r^{(i)} + e_{r-1}^{(i+1)}, \quad r = 1, \dots, M, \quad i = 0, \dots, 2M - 2r, \quad (4.77)$$

$$q_r^{(i)} = q_{r-1}^{(i+1)} e_{r-1}^{(i+1)} / e_{r-1}^{(i)}, \quad r = 2, \dots, M, \quad i = 0, \dots, 2M - 2r - 1. \quad (4.78)$$

We form the array

$$\begin{array}{ccccccc} & & & & & & q_1^{(0)} \\ & & & & & & e_1^{(0)} \\ e_0^{(1)} & & & & & & q_1^{(1)} & & q_2^{(0)} \\ & & & & & & e_1^{(1)} & & e_2^{(0)} \\ e_0^{(2)} & & & & & & q_1^{(2)} & & q_2^{(1)} \\ & & & & & & e_1^{(2)} & & \\ e_0^{(3)} & & & & & & q_1^{(3)} & & \\ & & & & & & e_1^{(3)} & & \\ e_0^{(4)} & & & & & & q_1^{(4)} & & \end{array}$$

The continued fraction coefficients d_k are given by $d_0 = a_0$ and

$$d_{2k-1} = -q_k^{(0)}, \quad d_{2k} = -e_k^{(0)}, \quad k = 1, \dots, M.$$

The qd -algorithm involves approximately the same amount of computational effort as the epsilon algorithm but does not need to be redone for each value of z . The successive convergents can be evaluated from (11.70) and (11.70a) by taking $p_0 = 0$, $p_1 = d_0$ and $q_0 = 1$, $q_1 = 1$ and letting $p_k = d_{k+1}z$, $q_k = 1$, $k \geq 2$ which de Hoog et al give in the equivalent form

$$A_{-1} = 0, \quad B_{-1} = 1, \quad A_0 = d_0, \quad B_0 = 1$$

$$\left. \begin{aligned} A_n &= A_{n-1} + d_n z A_{n-2} \\ B_n &= B_{n-1} + d_n z B_{n-2} \end{aligned} \right] n = 1, \dots, 2M$$

giving finally

$$v_{2M}(z) = A_{2M}/B_{2M}.$$

The estimate for $f(t)$ is then

$$\tilde{f}(t) = \frac{e^{\gamma t}}{T} \Re \left\{ \frac{A_{2M}}{B_{2M}} \right\}. \quad (4.79)$$

In addition to applying an acceleration procedure to the power series (4.76) they also apply an acceleration procedure to the continued fraction. This is achieved by writing

$$v(z) = \frac{d_0}{1+} \frac{d_1 z}{1+} \dots \frac{d_n z}{(1+r_{n+1})},$$

where $r_{n+1}(z)$ is the remainder. Usually, when evaluating the n th convergent A_n/B_n , we take r_{n+1} zero but we can evaluate $v(z)$ more accurately if we can get a better estimate for the remainder. The simplest assumption that we can make is that $d_{n+m} = d_{n+1}$ for all $m \leq 1$ which gives

$$r_{n+1} = d_{n+1} z / (1 + r_{n+1}).$$

As many continued fractions exhibit the pattern that coefficients repeat themselves in pairs, i.e.

$$d_{n+2m} = d_n, \quad d_{n+2m+1} = d_{n+1}, \quad m \geq 0,$$

this leads to a remainder estimate r'_{n+1} satisfying

$$r'_{n+1} = d_{n+1} z / (1 + d_n z / (1 + r'_{n+1})),$$

or

$$r'^2_{n+1} + [1 + (d_n - d_{n+1})z]r'_{n+1} - d_{n+1}z = 0.$$

For convergence we need to determine the root of smaller magnitude which is

$$r'_{n+1}(z) = -h_{n+1}[1 - (1 + d_{n+1}z/h_{n+1}^2)^{1/2}], \quad (4.80)$$

where $h_{n+1} = \frac{1}{2}[1 + (d_n - d_{n+1})z]$ and the complex square root has argument $\leq \pi/2$. The further improvement in convergence acceleration is obtained by computing A_k, B_k as before for $k = 1, \dots, 2M - 1$ and then computing

$$A'_{2M} = A_{2M-1} + r'_{2M}A_{2M-2}, \quad B'_{2M} = B_{2M-1} + r'_{2M}B_{2M-2}.$$

The computed estimate for $f(t)$ is then

$$\tilde{f}(t) = \frac{e^{\gamma t}}{T} \Re \left\{ \frac{A'_{2M}}{B'_{2M}} \right\}. \quad (4.81)$$

Honig and Hirdes [112] highlight a deficiency in all the above methods, namely, the dependence of the discretization and truncation errors on the free parameters. Suitable choice of these parameters can make the discretization error small but increase the truncation error and vice versa. They draw on the ‘Korrektur’ method of Albrecht and Honig [8] to reduce the discretization error without increasing the truncation error. Honig and Hirdes note that because the series (4.61) can only be summed to a finite number of terms (N) there also occurs a truncation error given by

$$E_T(N) = \frac{e^{ct}}{T} \left[\sum_{k=N+1}^{\infty} \left\{ \Re \bar{f} \left(c + i \frac{k\pi}{T} \right) \cos \frac{k\pi}{T} t - \Im \bar{f} \left(c + i \frac{k\pi}{T} \right) \sin \frac{k\pi}{T} t \right\} \right],$$

giving the approximate value of $f(t)$ as

$$f_N(t) = \frac{e^{ct}}{T} \left[-\frac{1}{2} \Re \bar{f}(c) + \sum_{k=0}^N \left\{ \Re \bar{f} \left(c + i \frac{k\pi}{T} \right) \cos \frac{k\pi}{T} t - \Im \bar{f} \left(c + i \frac{k\pi}{T} \right) \sin \frac{k\pi}{T} t \right\} \right]. \quad (4.82)$$

Equation (4.58) can now be written

$$f(t) = f_{\infty}(t) - E_3. \quad (4.83)$$

The ‘Korrektur’ method uses the approximation

$$f(t) = f_{\infty}(t) - e^{-2cT} f_{\infty}(2T+t) - E_4. \quad (4.84)$$

The approximate value of $f(t)$ is thus

$$\{f_N(t)\}_K = f_N(t) - e^{-2cT} f_{N_0}(2T+t). \quad (4.85)$$

The truncation error of the ‘Korrektur’ term $e^{-2cT} f_{\infty}(2T+t)$ is much smaller than $E_T(N)$ if $N = N_0$ which indicates that N_0 can be chosen less than N implying that just a few additional evaluations of $\bar{f}(s)$ will achieve a considerable reduction in the discretization error. Honig and Hirdes assert that the analysis in Albrecht and Honig enables one to show that

$$(a) \quad |E_4| \leq \frac{2\kappa}{e^{2cT}(e^{2cT} - 1)} \quad \text{if } m = 0, \quad (4.86)$$

$$(b) \quad |E_4| \leq 3^m e^{-2cT} \left\{ K(2T)^m e^{-2cT} \sum_{i=1}^{m+1} \frac{\alpha_i}{(2cT)^i} \right\}, \quad (4.87)$$

if $m > 0$ and $(m!)/2^m - 1 \leq 2cT$.

Honig and Hirdes outline the three acceleration methods used in the Fortran subroutine LAPIN which is given as an Appendix to their paper. These are the ϵ -algorithm (see §11.4) and the minimum-maximum method which are applied when the function $f_N(t)$ is non-monotonic and the curve fitting method when $f_N(t)$ is monotonic, which is to be understood in the sense that

$$|f_N(t) - f_\infty(t)| \geq |f_M(t) - f_\infty(t)|, \quad t \text{ fixed}$$

for all N, M with $N \leq M$. The minimum-maximum method consists of finding three neighbouring stationary values of $f_N(t)$ as a function of N , say a maximum at $N = N1$ and $N = N3$ and a minimum at $N = N2$. Linear interpolation is then used to find the value of f_{int} at $N = N2$ given the data pairs $(N1, f_{N1}(t))$ and $(N3, f_{N3}(t))$ and the mean value $(f_{int} + f_{N2}(t))/2$ is computed. This yields a new approximation for $f_\infty(t)$.

The curve fitting method consists in fitting the parameters of any function that has a horizontal asymptote $y = \zeta$ by demanding that this function is an interpolating function for the points $(N, f_N(t))$, $0 \leq N_0 \leq N \leq N_1$. The function value of the asymptote ζ is the desired approximation for $f(t)$. The use of the simple rational function

$$f_N(t) = \frac{\xi}{N^2} + \frac{\eta}{N} + \zeta, \quad (4.88)$$

is reported as giving high accuracy for small N_1 .

Honig and Hirdes give two methods for choosing optimal parameters N and cT and the reader should consult this paper as poor choice of the parameters will not improve the results. They also give a specification of the variables which are required to operate their subroutine LAPIN — the program and a digest of the specification can be downloaded from www.cf.ac.uk/maths/cohen/programs/inverselaplace/transform/.

4.5 Hartley Transforms

Hwang, Lu and Shieh [114], following the approach in the previous section, approximate the integral in

$$f(t) = \frac{e^{ct}}{2\pi} \int_{-\infty}^{\infty} \bar{f}(c + i\omega) e^{i\omega t} d\omega,$$

by applying the trapezium rule for integration with $\omega = k\pi/mT$ and $\Delta\omega = \pi/mT$ where m is a positive integer ($m = 1$ previously). They thus obtain

$$f(t) \approx \frac{e^{ct}}{2mT} \sum_{k=-\infty}^{\infty} \bar{f}\left(c + i\frac{k\pi}{mT}\right) \exp\left(i\frac{k\pi}{mT}t\right). \quad (4.89)$$

This last result can be written as

$$f(t) \approx \frac{e^{ct}}{2mT} \sum_{k=-M}^M \bar{f} \left(c + i \frac{k\pi}{mT} \right) \exp \left(i \frac{k\pi}{mT} t \right) + e^{ct} E, \quad (4.90)$$

where E is the truncation error and M is a positive integer which is chosen so that $e^{ct}E$ is negligible compared with $f(t)$.

If we let $t = q\Delta T$, $\Delta T = 2T/N$, $M = mnN/2 + [(m-1)/2]$ with N a positive power of 2, then (4.90) can be rewritten as

$$f(q\Delta T) = \frac{e^{cq\Delta T}}{2mT} \left(W^{N/2} \right)^{qn} \sum_{r=-m_1}^{m_2} W^{qr/m} \left\{ \sum_{k=0}^{N-1} \bar{f}_r(k) W^{qk} \right\} \quad (4.91)$$

$$= (-1)^{qn} \frac{e^{qc\Delta T}}{2mT} \sum_{r=-m_1}^{m_2} W^{qr/m} \left\{ \sum_{k=0}^{N-1} \widehat{\bar{f}_r(k)} W^{-qk} \right\} \quad (4.92)$$

where \widehat{z} denotes the complex conjugate of z , $[x]$ the integer part of x and

$$m_1 = \left[\frac{m-1}{2} \right], \quad (4.93)$$

$$m_2 = \begin{cases} m_1 & \text{for } m \text{ odd} \\ m_1 + 1 & \text{for } m \text{ even} \end{cases} \quad (4.94)$$

$$W = \exp \left(i \frac{2\pi}{N} \right) \quad (4.95)$$

$$\bar{f}_r(k) = \sum_{p=0}^{n_1} \bar{f} \left(c + i \frac{\pi}{T} \left(k + \frac{r}{m} + \frac{N}{2} (2p-n) \right) \right), \quad k = 0, 1, \dots, N-1 \quad (4.96)$$

and

$$n_1 = \begin{cases} n & k = 0 \text{ and } r \neq m/2 \\ n-1 & \text{otherwise} \end{cases} \quad (4.97)$$

From (4.92) the value of $f(q\Delta T)$, $q = 0, 1, \dots, N-1$ can be obtained by m sets of N -point FFT computations. After selecting appropriate values of c, T, m, n and N we can compute $\bar{f}_r(k)$ from $\bar{f}(s)$ using (4.96). Let

$$f_r(q) = \sum_{k=0}^{N-1} \widehat{\bar{f}_r(k)} W^{-qk}, \quad q = 0, 1, \dots, N-1 \quad (4.98)$$

Then

$$\{\widehat{\bar{f}_r(k)}\} \xrightarrow{FFT} \{f_r(q)\},$$

and the inverse function $f(t)$ at $t = q\Delta T$ is determined from

$$f(q\Delta T) = (-1)^{qn} \frac{e^{cq\Delta T}}{2mT} \sum_{r=-m_1}^{m_2} W^{qr/m} \widehat{f_r(q)}, \quad q = 0, 1, \dots, N-1 \quad (4.99)$$

On account of the method of construction of (4.90) a relationship exists between $\bar{f}_r(k)$ and $\bar{f}_{-r}(k)$ and one does not have to perform m sets of N -point FFT computations. First note that $\widehat{\bar{f}(c+i\omega)} = \widehat{\bar{f}(c-i\omega)}$. Then, from (4.96) we have the following properties of $\bar{f}_r(k)$:-

$$\left. \begin{aligned} \bar{f}_0(k) &= \left\{ \begin{array}{ll} \text{real} & k = 0, N/2 \\ \bar{f}_0(\overline{N-k}) & k = 1, 2, N/2 - 1 \end{array} \right\} \\ \bar{f}_r(k) &= \bar{f}_{-r}(\overline{N-k}) & r = 1, 2, \dots, m_1 \\ \bar{f}_r(k) &= \bar{f}_{-r}(N-k-1) & k = 0, 1, \dots, N/2 - 1, r = m/2, m \text{ even} \end{aligned} \right\} \quad (4.100)$$

Applying these results in conjunction with (4.98) shows that the transformed sequence $\{f_r(q)\}$ has the following properties:-

$$\left. \begin{aligned} f_0(q) &= \text{real} & q = 0, 1, \dots, N-1 \\ f_r(q) &= \bar{f}_{-r}(q) & q = 0, 1, \dots, N-1 \\ \Im\{f_r(q)W^{q/2}\} &= 0 & q = 1, \dots, N-1, r = m/2, m \text{ even} \end{aligned} \right\} \quad (4.101)$$

Thus in order to obtain $f(t)$ at $t = q\Delta T$, $q = 0, 1, \dots, N-1$ only $m_2 + 1$ sets of N -point FFT computations are required. Suppose the computed sequences are $\{f_r(q)\}$ for $r = 0, 1, \dots, m_2$. Then

$$f(q\Delta T) \approx (-1)^{qm} \frac{e^{cq\Delta T}}{2mT} \tilde{f}(q) \quad (4.102)$$

where

$$\tilde{f}(q) = \left\{ \begin{array}{ll} f_0(q) + 2 \sum_{r=1}^{m_1} [\Re\{f_r(q)\} \cos(\frac{2\pi qr}{mN}) - \Im\{f_r(q)\} \sin(\frac{2\pi qr}{mN})] & m = \text{odd} \\ f_0(q) + 2 \sum_{r=1}^{m_1} [\Re\{f_r(q)\} \cos(\frac{2\pi qr}{mN}) - \Im\{f_r(q)\} \sin(\frac{2\pi qr}{mN})] \\ \quad + \Re\{f_{m_2}(q)\} \cos(\pi q/N) & m = \text{even} \end{array} \right. \quad (4.103)$$

We now illustrate how the above FFT inversion formula (4.92) can be evaluated by using multiple sets of N -point FHT computations (see Appendix 11.2). First let

$$h_r(q) = \sum_{k=0}^{N-1} H_r(q) \text{cas}(2\pi kq/N), \quad (4.104)$$

and denote the above transform by

$$\{H_r(k)\} \xrightarrow{FHT} \{h_r(q)\}. \quad (4.105)$$

If $\{H(k)\}$ and $\{h(q)\}$ are discrete Hartley transform pairs and $\{\bar{f}(k)\}$ and $\{f(q)\}$ are discrete Fourier transform pairs and, in addition, $H(k)$ and $\bar{f}(k)$ are related by

$$H(k) = \Re\{\bar{f}(k)\} - \Im\{\bar{f}(k)\}, \quad k = 0, 1, \dots, N-1 \quad (4.106)$$

then

$$h(q) = \Re\{f(q)\} + \Im\{f(N - q)\}, \quad k = 0, 1, \dots, N - 1 \quad (4.107)$$

Hwang et al define $H_r(k)$ by

$$H_r(k) = \begin{cases} \Re\{\bar{f}_0(k)\} - \Im\{\bar{f}_0(k)\} & r = 0, \\ & k = 0, 1, \dots, N/2 - 1 \\ \Re\{\bar{f}_0(N - k)\} + \Im\{\bar{f}_0(N - k)\} & r = 0, \\ & k = N/2, N/2 + 1, \dots, N - 1 \\ \Re\{\bar{f}_r(k)\} - \Im\{\bar{f}_r(k)\} & r = 1, 2, \dots, m_1, \\ & k = 1, 2, \dots, N - 1 \\ \Re\{\bar{f}_{-r}(N - k)\} + \Im\{\bar{f}_{-r}(N - k)\} & r = -1, -2, \dots, -m_1, \\ & k = 0, 1, \dots, N - 1 \\ \Re\{\bar{f}_r(k)\} - \Im\{\bar{f}_r(k)\} & r = m/2, m \text{ even} \\ & k = 0, 1, \dots, N/2 - 1 \\ \Re\{\bar{f}_r(N - k - 1)\} + \Im\{\bar{f}_r(N - k - 1)\} & r = m/2, m \text{ even} \\ & k = N/2, N/2 + 1, \dots, N - 1 \end{cases} \quad (4.108)$$

From (4.100) it follows that $H_r(k)$ and $\bar{f}_r(k)$ satisfy the relation (4.106) and thus $h_r(q)$ and $f_r(q)$ are related by

$$h_r(q) = \Re\{f_r(q)\} + \Im\{f_r(N - q)\} \quad \begin{array}{l} \text{for } q = 0, 1, \dots, N - 1 \\ r = -m_1, -m_1 + 1, \dots, m_2 \end{array} \quad (4.109)$$

Since $\widehat{f_r(q)} = f_{-r}(q)$, we have

$$h_0(q) = f_0(q) \quad \text{for } q = 0, 1, \dots, N - 1 \quad (4.110)$$

$$\begin{aligned} h_{-r}(q) &= \Re\{f_{-r}(q)\} + \Im\{f_{-r}(N - q)\} \\ &= \Re\{f_r(q)\} + \Im\{f_r(N - q)\} \quad \text{for } r = 1, 2, \dots, m_1 \end{aligned} \quad (4.111)$$

It follows that

$$\Re\{f_r(q)\} = \frac{1}{2}[h_r(q) + h_{-r}(q)] \quad (4.112)$$

and

$$\Im\{f_r(q)\} = \frac{1}{2}[h_r(N - q) - h_{-r}(N - q)] \quad (4.113)$$

for $q = 0, 1, \dots, N - 1$ and $r = 0, 1, \dots, m_1$. Finally, we have the FHT expressions for $f(t)$ at $t = q\Delta T$,

$$\begin{aligned} f(q\Delta T) &\approx (-1)^{nq} \frac{e^{cq\Delta T}}{2mT} \left(h_0(q) + \sum_{r=1}^{m_1} \left([h_r(q) + h_{-r}(q)] \cos \frac{2\pi qr}{mN} \right. \right. \\ &\quad \left. \left. - [h_r(N - q) - h_{-r}(N - q)] \sin \frac{2\pi qr}{mN} \right) \right) \quad m \text{ odd} \end{aligned} \quad (4.114)$$

$$\begin{aligned}
f(q\Delta T) \approx & (-1)^{nq} \frac{e^{cq\Delta T}}{2mT} \left(h_0(q) + \sum_{r=0}^{m_1} \left([h_r(q) + h_{-r}(q)] \cos \frac{2\pi qr}{mN} \right. \right. \\
& \left. \left. - [h_r(N-q) + h_{-r}(N-q)] \sin \frac{2\pi qr}{mN} \right) \right. \\
& \left. + h_{m/2}(q) \cos \frac{\pi q}{N} - h_{m/2}(N-q) \sin \frac{\pi q}{N} \right) \quad m \text{ even}
\end{aligned} \tag{4.115}$$

Hwang, Wu and Lu [115] note that $\mathcal{L}^{-1}\{\bar{f}^{(n)}(s)\} = (-1)^n t^n f(t)$ and find that with their test examples they get superior results by using the FHT method applied to $f''(s)$.

4.6 Dahlquist's "Multigrid" extension of FFT

Dahlquist [55] noted that the Discrete Fourier Transform (DFT) is often an efficient device for the numerical computation of Fourier integrals, particularly with a Fast Fourier Transform (FFT) implementation. However, if $\mathfrak{F}(\omega)$ is singular or nearly singular at $\omega = 0$ as well as slowly decreasing as $\omega \rightarrow \infty$, the number of function values required can become prohibitively large. Thus it would be advantageous to have some scheme with a variable step size.

Suppose that $[-t', t']$, $[-\omega', \omega']$ are the shortest intervals on the t and ω axes respectively that have to be covered in order to meet accuracy requirements and N is the number of sub-intervals on a grid on each of these intervals. The highest frequency that can be resolved by the grid on the t -axis is then $\omega' = \pi/\Delta t = \pi N/2t'$. Hence $\frac{1}{2}N \geq t'\omega'/\pi$. However, Dahlquist finds it more convenient to choose equality so that, if $N' = \frac{1}{2}N$,

$$\pi N' = t'\omega'. \tag{4.116}$$

Dahlquist observes that if we want to compute $f(t)$ to d decimal places when

$$\mathfrak{F}(\omega) = (\sigma + i\omega)^{-k} \phi(\omega), \tag{4.117}$$

and $\phi(\omega)$ is a slowly varying function such that $\phi(\omega) \approx 1$ for large and small values of ω , then $N' = \max \omega/\Delta\omega$, for a straightforward application of the DFT. A reasonable choice is $\Delta\omega \approx 0.1\sigma$. The choice of $\max \omega$ if we desire that the error in $f(t)$ on the whole real axis should be less than 10^{-d} is, applying criteria formulated by Dahlquist, given by $\max \omega^{1-k}/(k-1) = 10^{-d}$. If this accuracy is required only for $|t| \geq \delta$ then we have instead

$$(2/\pi)\delta^{-2}k \max \omega^{-1-k} = 10^{-d}.$$

The implications of the above are that with $\sigma = 0.01$, $k = 1.5$, and $d = 5$ we have $\Delta\omega \approx 0.001$ and about $4 \cdot 10^{13}$ function values are needed for a DFT in the first case. With $\delta = 10^{-4}$ about $2 \cdot 10^8$ values are needed in the second case. Clearly the difficulty in the above example is the vast number of function evaluations to be performed. However, for functions like $\mathfrak{F}(\omega)$ defined by (4.117), where

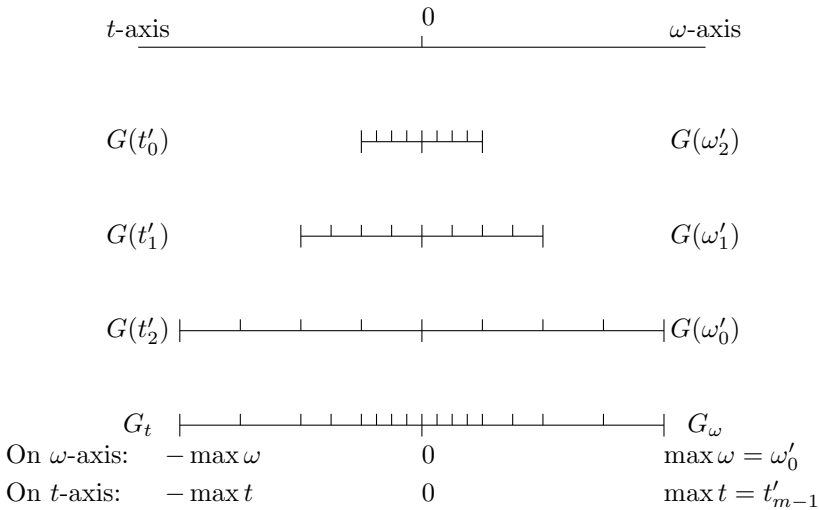


Figure 4.3: The structure of the grids used in the algorithm

it is reasonable to interpolate on some equidistant *logarithmic* grid, Dahlquist presents an algorithm which has some of the advantages of FFT and which can be implemented to invert the Laplace transform. The number of function values now required is of the order of 1000 which is much more manageable.

The algorithm works with the same N on m grids on the ω -axis, and m corresponding grids on the t -axis. On the ω -axis Dahlquist chooses

$$\omega' = \omega'_0, \omega'_1, \dots, \omega'_{m-1}, \quad \text{where } \omega'_0 = \max \omega, \quad \omega'_j = \omega'_{j-1}/2. \quad (4.118)$$

Similarly, on the t -axis we choose,

$$t' = t'_0, t'_1, \dots, t'_{m-1}, \quad t'_j = \pi N' / \omega'_j, \quad \text{hence } t'_j = 2t'_{j-1}. \quad (4.119)$$

$G(t')$ denotes the grid with $N + 1$ equidistant points on the interval $[-t', t']$ and $G(\omega')$ has a similar connotation. We set

$$G_\omega = \bigcup_{j=0}^{m-1} G(\omega'_j), \quad G_t = \bigcup_{j=0}^{m-1} G(t'_j). \quad (4.120)$$

Thus in figure 4.3 we have illustrated the case $m = 3$, $N = 8$ although more typical values would be $m = 20$, $N = 128$. Dahlquist notes that the sets G_ω and G_t are similar in structure to the set of floating point numbers. Locally they are equidistant while globally they are more like being equidistant on a

logarithmic scale. We can be more precise about the number of function values required which is $N'(m+1)/2$, which is less than $N' \log_2(\max \omega / \min \Delta \omega)$. Having dispensed with the preliminaries relating to the grid we now give the basis of Dahlquist's algorithm which is a generalization of Poisson's summation formula and is stated in Theorem 4.1

Theorem 4.1 *Assume that $\mathfrak{F}(\omega)$ is continuous and absolutely integrable over $(-\infty, \infty)$ and $\mathfrak{F}'(\omega)$ is continuous, except for a finite number of jump discontinuities. Let $f(t)$ be the inverse Fourier transform of $\mathfrak{F}(\omega)$. Let t', ω' be positive constants and define the periodic functions*

$$\mathfrak{F}(\omega, \omega') = \sum_{r=-\infty}^{\infty} \mathfrak{F}(\omega + 2r\omega'), \quad f(t, t') = \sum_{m=-\infty}^{\infty} f(t + 2mt'). \quad (4.121)$$

The construction implies that $\mathfrak{F}(\omega, \omega')$ is determined everywhere by its values for $|\omega| \leq \omega'$ and similarly $f(t, t')$ is determined by its values for $|t| \leq t'$. Assume that the expansion defining $\mathfrak{F}(\omega, \omega')$ is absolutely and uniformly convergent for every $\omega' > 0$, and the same holds for $\mathfrak{F}'(\omega, \omega')$ if some neighbourhoods of the discontinuities have been excluded.

Let N be a natural number and set

$$N' = N/2, \quad \Delta\omega = \omega'/N', \quad t'\omega' = \pi N', \quad \Delta t = t'/N'. \quad (4.122)$$

These equations also imply

$$\Delta\omega = \pi/t', \quad \Delta t = \pi/\omega', \quad \Delta\omega\Delta t = \pi/N'. \quad (4.122')$$

Then the expansion for $f(t, t')$ is absolutely convergent for all t , and the discrete Fourier transform gives

$$\mathfrak{F}(r\Delta\omega, \omega') = \Delta t \sum_{k=0}^{N-1} f(k\Delta t, t') e^{-2\pi i r k / N}, \quad r = 0, 1, \dots, N-1. \quad (4.123)$$

■

The inverse DFT yields,

$$f(k\Delta t, t')\Delta t = \frac{1}{N} \sum_{r=0}^{N-1} \mathfrak{F}(r\Delta\omega, \omega') e^{2\pi i r k / N}, \quad k = 0, 1, \dots, N-1.$$

This can also be written as

$$f(k\Delta t, t') = \frac{\Delta\omega}{2\pi} \sum_{r=0}^{N-1} \mathfrak{F}(r\Delta\omega, \omega') e^{2\pi i r k / N}, \quad k = 0, 1, \dots, N-1, \quad (4.124)$$

by virtue of (4.122) and (4.122'). Note that because of the periodicity of $f(t, t')$ we can consider the first argument to be reduced modulo $2t'$ so that it lies in

the interval $[-t', t']$. Similarly for $\mathfrak{F}(\omega, \omega')$.

An important property of $f(t, t')$ is that

$$f(t, t') = \sum_{j=-\infty}^{\infty} f(t + 4jt') + \sum_{j=-\infty}^{\infty} f(t - 2t' + 4jt'),$$

or

$$f(t, t') = f(t, 2t') + f(t - 2t', 2t'). \quad (4.125)$$

Likewise,

$$\mathfrak{F}(\omega, \omega') = \mathfrak{F}(\omega, 2\omega') + \mathfrak{F}(\omega - 2\omega', 2\omega'). \quad (4.125')$$

Thus if the $4\omega'$ -periodic function $\mathfrak{F}(\cdot, 2\omega')$ is known on $G(2\omega')$ then $\mathfrak{F}(\omega, \omega')$ is directly determined for $\omega \in G(2\omega')$, but for $\omega \in G(\omega') \setminus G(2\omega')$ some interpolation is necessary. This can be achieved by subtracting $\mathfrak{F}(\omega)$ from both sides of (4.125') to get

$$\mathfrak{F}(\omega, \omega') - \mathfrak{F}(\omega) = (\mathfrak{F}(\omega, 2\omega')) + \mathfrak{F}(\omega - 2\omega', 2\omega'). \quad (4.126)$$

If now $|\omega| \leq \omega'$ then, by the definition of the $2\omega'$ -periodic function $\mathfrak{F}(\cdot, \omega')$, it follows that the left hand side of (4.126) depends only on values of $\mathfrak{F}(\omega)$ with $|\omega| > \omega'$. This is also the case for the right hand side.

Dahlquist now assumes that \mathfrak{F} can be approximated with sufficient accuracy by a piecewise cubic spline \mathfrak{G} with the following properties:-

A. $\mathfrak{G}(\omega) = 0$ for $|\omega| > \omega'_0$ (The largest ω' in the sequence).

B. For $j = 1, 2, \dots, m-1$, $\mathfrak{G}(\omega)$ is, for $\omega'_j < \omega < 2\omega'_j$, a cubic spline determined by interpolation of $\mathfrak{F}(\omega)$ at $\omega = \omega'_j + 2k\omega'_j/N'$, $k = 0, 1, \dots, N'/2$, with “not a knot conditions” at $k = 1$ and $k = N'/2 - 1$, (DeBoor [63]). Similarly for $-2\omega'_j < \omega < -\omega'_j$ — the accuracy of this interpolation is $O(N^{-4})$.

We now have the algorithm (where \mathfrak{F} has to be understood as \mathfrak{G}).

ALGORITHM I: Construction of $\mathfrak{F}(\omega, \omega')$, $\omega' = \omega'_0, \omega'_1, \dots, \omega'_{m-1}$, and computation of $f(t, t')$ by the FFT.

1. Compute $\mathfrak{F}(\omega, \omega'_0) = \mathfrak{F}(\omega)$, $\omega \in G(\omega'_0)$.
2. Set $t_0 = \pi N'/\omega'_0$.
3. Compute $f(t, t'_0)$ by the FFT from (4.124), $t \in G(t_0)$.
4. For $\omega' = \omega'_1, \omega'_2, \dots, \omega'_{m-1}$, do:
5. Compute $\mathfrak{F}(\omega, \omega') - \mathfrak{F}(\omega)$, from (4.126), $\omega \in G(2\omega')$.
6. Interpolate the result from $G(2\omega')$ to $G(\omega') \setminus G(2\omega')$.
7. Compute $\mathfrak{F}(\omega, \omega') = \mathfrak{F}(\omega) + (\mathfrak{F}(\omega, \omega') - \mathfrak{F}(\omega))$, $\omega \in G(\omega')$.
8. Set $t = \pi N'/\omega$.
9. Compute $f(t, t')$ by the FFT, from (4.126), $t \in G(t')$, where

$$G(t') = \{t = kt'/N', \quad k = 0, \pm 1, \pm 2, \dots, \pm N'\}.$$

End.

In order to complete the process and reconstruct $f(t)$ from the $2t'$ -periodic function $f(t, t')$, $t' = t'_{m-1}, t'_{m-2}, \dots, t'_0$ we need the analogue of (4.126), namely

$$f(t, t') - f(t) = (f(t, 2t') - f(t)) + f(t - 2t', 2t'), \quad (4.126')$$

and the assumption that $f(t)$ can be replaced by a function $g(t)$ with the properties:

A*. $g(t) = 0$ for $|t| > t'_{m-1}$;

B*. For $j = 0, 1, \dots, m-2$, $g(t)$ is, for $t'_j < t < 2t'_j$ a cubic spline determined by the interpolation at $t = t'_j + 2kt'_j/N'$, $k = 0, 1, \dots, N'/2$, with "not a knot conditions" at $k = 1$ and $k = N'/2 - 1$. Similarly for $-2t'_j < t < -t'_j$.

This leads to the following algorithm (where again f is used instead of g).

ALGORITHM II: Reconstruction of $f(t)$ from $f(t, t')$, $t = t'_{m-1}, t'_{m-2}, \dots, t'_0$.

1. Compute $f(t) = f(t, t'_{m-1})$, $t \in G(t'_{m-1})$.
2. For $t' = t'_{m-2}, t'_{m-3}, \dots, t'_0$, do:
3. Compute $f(t, t') - f(t)$ from (4.126'), $t \in G(2t')$.
4. Interpolate the result from $G(2t')$ to $G(t') \setminus G(2t')$.
5. Compute $f(t) = f(t, t') - (f(t, t') - f(t))$, $t \in G(t') \setminus G(2t')$.

End.

Dahlquist gives details of the practicalities involved in implementing the algorithms, which we shall omit here, before proceeding to the application of finding the inverse Laplace transform. He writes

$$\bar{g}(s) = \int_0^\infty e^{-st} g(t) dt, \quad s = \sigma + i\omega, \quad (4.127)$$

where $g(t)$ is a real function. Thus

$$\Re \bar{g}(s) = \int_0^\infty \cos(\omega t) e^{-\sigma t} g(t) dt. \quad (4.127')$$

Now assume that $\Re \bar{g}(s)$ satisfies sufficient conditions for the validity of the inverse cosine transform formula. Then

$$e^{-\sigma t} g(t) = \frac{2}{\pi} \int_0^\infty \cos(\omega t) \Re \bar{g}(s) d\omega, \quad t > 0. \quad (4.128)$$

If we set

$$\mathfrak{F}(\omega) = 2\Re \bar{g}(s), \quad f(t) = e^{-\sigma|t|} g(|t|) \quad (4.129)$$

then we can rewrite (4.128) in the form

$$f(t) = \frac{1}{2\pi} \int_{-\infty}^\infty e^{i\omega t} \mathfrak{F}(\omega) d\omega, \quad (4.128')$$

which is valid for all real t . This last integral has to be interpreted as a Cauchy principal value, i.e.,

$$\int_{-\infty}^\infty = \lim_{T \rightarrow \infty} \int_{-T}^T.$$

The above re-formulation has transformed the problem to one in which the Algorithms I and II are applicable — see Dahlquist for further particulars.

4.7 Inversion of two-dimensional transforms

We have seen earlier in this Chapter that Fourier series approximation provides an efficient technique for evaluating the inverse transform in one dimension. Moorthy [158] has extended this technique to two dimensions — the extension to higher dimensions also being possible.

If $|f(t_1, t_2)| < Me^{\gamma_1 t_1 + \gamma_2 t_2}$ and we define

$$\bar{f}(s_1, s_2) = \int_0^\infty \int_0^\infty e^{-s_1 t_1 - s_2 t_2} f(t_1, t_2) dt_1 dt_2 \quad \Re s_1 > \gamma_1, \Re s_2 > \gamma_2 \quad (4.130)$$

then the inverse transform can be expressed as

$$f(t_1, t_2) = \frac{1}{(2\pi i)^2} \int_{c_1 - i\infty}^{c_1 + i\infty} \int_{c_2 - i\infty}^{c_2 + i\infty} e^{s_1 t_1 + s_2 t_2} \bar{f}(s_1, s_2) ds_1 ds_2, \quad (4.131)$$

where $c_1 > \gamma_1$ and $c_2 > \gamma_2$. Equation (4.131) can be rewritten as

$$\begin{aligned} f(t_1, t_2) = \frac{e^{c_1 t_1 + c_2 t_2}}{4\pi^2} \left\{ \int_{-\infty}^\infty \int_{-\infty}^\infty [\Re \bar{f}(c_1 + i\omega_1, c_2 + i\omega_2) \cos(\omega_1 t_1 + \omega_2 t_2) \right. \\ \left. - \Im \bar{f}(c_1 + i\omega_1, c_2 + i\omega_2) \sin(\omega_1 t_1 + \omega_2 t_2)] d\omega_1 d\omega_2 \right\} \end{aligned} \quad (4.132)$$

This can be rewritten as

$$\begin{aligned} f(t_1, t_2) = \frac{e^{c_1 t_1 + c_2 t_2}}{2\pi^2} \left\{ \int_{-\infty}^\infty \int_{-\infty}^\infty [\Re \bar{f}(c_1 + i\omega_1, c_2 + i\omega_2) \cos(\omega_1 t_1 + \omega_2 t_2) \right. \\ \left. - \Im \bar{f}(c_1 + i\omega_1, c_2 + i\omega_2) \sin(\omega_1 t_1 + \omega_2 t_2)] d\omega_1 d\omega_2 \right. \\ \left. + \int_{-\infty}^\infty \int_{-\infty}^\infty [\Re \bar{f}(c_1 + i\omega_1, c_2 - i\omega_2) \cos(\omega_1 t_1 - \omega_2 t_2) \right. \\ \left. - \Im \bar{f}(c_1 + i\omega_1, c_2 - i\omega_2) \sin(\omega_1 t_1 - \omega_2 t_2)] d\omega_1 d\omega_2 \right\}. \end{aligned} \quad (4.133)$$

Moorthy defines a function $g^{jk}(t_1, t_2)$ with the property that

$$g^{jk}(t_1, t_2) = e^{-(c_1 t_1 + c_2 t_2)} f(t_1, t_2) \quad \text{in} \quad (2jT, 2(j+1)T) \times (2kT, 2(k+1)T),$$

and elsewhere it is periodic with period $2T$ in t_1 and t_2 . Thus g^{jk} has Fourier series representation given by

$$\begin{aligned} g^{jk}(t_1, t_2) = \frac{1}{4} a_{00}^{jk} + \frac{1}{2} \sum_{m=1}^\infty (a_{0m}^{jk} \cos my + b_{0m}^{jk} \sin my) \\ + \frac{1}{2} \sum_{n=1}^\infty (a_{n0}^{jk} \cos nx + c_{n0}^{jk} \sin nx) \\ + \frac{1}{2} \sum_{n=1}^\infty \sum_{m=1}^\infty (a_{nm}^{jk} \cos nx \cos my + b_{nm}^{jk} \cos nx \sin my \\ + c_{nm}^{jk} \sin nx \cos my + d_{nm}^{jk} \sin nx \sin my), \end{aligned}$$

where $x = \pi t_1/T$, $y = \pi t_2/T$, and, typically,

$$a_{nm}^{jk} = \frac{1}{T^2} \int_{2jT}^{2(j+1)T} \int_{2kT}^{2(k+1)T} f(u, v) \cos(n\pi u/T) \cos(m\pi v/T) e^{-c_1 u - c_2 v} du dv,$$

with similar expressions for b_{nm}^{jk} , c_{nm}^{jk} , d_{nm}^{jk} . Substituting for the a, b, c, d in $g^{jk}(t_1, t_2)$ and summing over j, k Moorthy obtained, after interchanging the order of summation

$$\begin{aligned} & \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} g^{jk}(t_1, t_2) \\ &= \frac{1}{2T^2} \left\{ \frac{1}{2} \bar{f}(c_1, c_2) + \sum_{m=1}^{\infty} \left[\Re \bar{f} \left(c_1, c_2 + \frac{im\pi}{T} \right) \cos \left(\frac{m\pi t_2}{T} \right) \right. \right. \\ & \quad \left. \left. - \Im \bar{f} \left(c_1, c_2 + \frac{im\pi}{T} \right) \sin \left(\frac{m\pi t_2}{T} \right) \right] \right. \\ & \quad + \sum_{n=1}^{\infty} \left[\Re \bar{f} \left(c_1 + \frac{in\pi}{T}, c_2 \right) \cos \left(\frac{n\pi t_1}{T} \right) \right. \\ & \quad \left. \left. - \Im \bar{f} \left(c_1 + \frac{in\pi}{T}, c_2 \right) \sin \left(\frac{n\pi t_1}{T} \right) \right] \right. \\ & \quad + \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \left[\Re \bar{f} \left(c_1 + \frac{in\pi}{T}, c_2 \pm \frac{im\pi}{T} \right) \cos \left(\frac{n\pi t_1 \pm m\pi t_2}{T} \right) \right. \\ & \quad \left. \left. - \Im \bar{f} \left(c_1 + \frac{in\pi}{T}, c_2 \pm \frac{im\pi}{T} \right) \sin \left(\frac{n\pi t_1 \pm m\pi t_2}{T} \right) \right] \right\}. \end{aligned} \tag{4.134}$$

If the sum on the right hand side of (4.134) is denoted by $g(t_1, t_2)$ then the approximate value of f on $(0, 2T) \times (0, 2T)$ is given by

$$\tilde{f}(t_1, t_2) = e^{c_1 t_1 + c_2 t_2} g(t_1, t_2).$$

Moorthy shows that the error in the approximation \tilde{f} can be reduced by taking $c_1 > \gamma_1$ and $c_2 > \gamma_2$. A suitable choice for T was found by experimentation to be such that $t_{\max} < 2T$ and $0.5t_{\max} < T \leq 0.8t_{\max}$. A further error is incurred in evaluating (4.134) as the best we can achieve is the evaluation of $g_N(t_1, t_2)$ and hence $\tilde{f}_N(t_1, t_2)$ where the summations in (4.134) have been limited to N terms. Control of the truncation error is obtained by choosing N such that the difference between $\tilde{f}_{N+1}(t_1, t_2)$ and $\tilde{f}_{N+N/4}(t_1, t_2)$ is negligible.

Chapter 5

Rational Approximation Methods

5.1 The Laplace Transform is Rational

If a given Laplace transform $\bar{f}(s)$ can be represented in the form $P(s)/Q(s)$ where $P(s)$ and $Q(s)$ are polynomials of degree p and q respectively with $p \leq q$, say,

$$\begin{aligned}P(s) &= s^p + a_1 s^{p-1} + \cdots + a_p, \\Q(s) &= s^q + b_1 s^{q-1} + \cdots + b_q,\end{aligned}$$

then the expansion theorem (1.23) or the theory of partial fractions informs us that if the roots of $Q(s) = 0$ are distinct

$$\bar{f}(s) = \frac{P(s)}{Q(s)} = A_0 + \frac{A_1}{s - \alpha_1} + \frac{A_2}{s - \alpha_2} + \cdots + \frac{A_q}{s - \alpha_q}, \quad (5.1)$$

where $\alpha_1, \alpha_2, \dots, \alpha_q$ are the roots of the equation $Q(s) = 0$ and A_0, A_1, \dots, A_q are constants. It is now very easy to determine $f(t)$ from the knowledge of the expansion (5.1) as

$$f(t) = A_0 \delta(t) + A_1 e^{\alpha_1 t} + A_2 e^{\alpha_2 t} + \cdots + A_q e^{\alpha_q t}. \quad (5.2)$$

If any of the roots of $Q(s) = 0$ are repeated then we have to modify (5.1) and (5.2).

Example 5.1 A Batch Service Queue Problem.

One approach to determining an approximation to the estimation of the mean number of customers in Application 1, §10.1, is by iterating rational approximations. Our initial approximation is

$$\bar{M}_1(s) = \frac{3}{s(s+1)}$$

which yields

$$M_1(t) = 3 - 3e^{-t},$$

After one iteration we have the approximation

$$\begin{aligned}\bar{M}_2(s) &\sim \frac{3(s+4)^2}{s(s^3+9s^2+24s+7)}, \\ &= \frac{48/7}{s} + \frac{\alpha}{(s-a)} - \frac{\beta(s-b)+\gamma c}{(s-b)^2+c^2},\end{aligned}$$

where $\alpha = -6.635827218$, $\beta = -0.2213156422$, $\gamma = -0.10313013323$, $a = -0.3313149094$, $b = -4.334342545$ and $c = 1.53016668458$. It follows that

$$M_2(t) = \frac{48}{7} + \alpha e^{at} + e^{bt}(\beta \cos ct + \gamma \sin ct).$$

After two iterations we have

$$\bar{M}_3(s) = \frac{p(s)}{q(s)},$$

where

$$\begin{aligned}p(s) &= 3(s+4)^2(s^3+12s^2+48s+55)(s^3+12s^2+48s+37) \\ q(s) &= s(s^9+33s^8+480s^7+3987s^6+20532s^5+66624s^4 \\ &\quad +132117s^3+146211s^2+71076s+4606).\end{aligned}$$

We can show that the roots of the denominator are $s = 0$ and

$$\begin{aligned}-5.5040122292 \pm 2.7546334460i &= a_1 \pm ib_1 \\ -5.0969767814 \pm 1.6328516314i &= a_2 \pm ib_2 \\ -4.1895509142 \pm 1.3080555188i &= a_3 \pm ib_3 \\ -1.6721845193 \pm 0.3992751935i &= a_4 \pm ib_4 \\ -0.0745511119 + 0.0000000000i &= a_5\end{aligned}$$

which enables us to determine the partial fraction representation of $\bar{M}_3(s)$, namely,

$$\bar{M}_3(s) = \frac{\alpha_5}{s-a_5} + \sum_{i=1}^4 \frac{\alpha_i(s-a_i) + \beta_i b_i}{(s-a_i)^2 + b_i^2} + \frac{48840}{2303s}$$

where

$$\begin{aligned}\alpha_1 &= -0.0247620331 & \beta_1 &= -0.013920958 \\ \alpha_2 &= 0.0022108833 & \beta_2 &= 0.047603163 \\ \alpha_3 &= -0.1670066287 & \beta_3 &= -0.154532492 \\ \alpha_4 &= -0.5637150577 & \beta_4 &= -0.324196946 \\ \alpha_5 &= -20.45384832\end{aligned}$$

It is now easy to determine the function corresponding to each Laplace transform. We have

$$M_3(t) = \alpha_5 e^{a_5 t} + \sum_{i=1}^4 e^{a_i t} (\alpha_i \cos b_i t + \beta_i \sin b_i t) + 21.20712115.$$

We can, of course, get the next approximation $M_4(t)$ in the same way but the expressions become horrendously complicated.

Longman and Sharir [145] have shown that partial fraction decomposition can be avoided. Consider first the special case where

$$\bar{f}(s) = \frac{1}{Q(s)},$$

then

$$\bar{f}(s) = \sum_{r=1}^q \frac{1}{Q'(\alpha_r)} \frac{1}{s - \alpha_r},$$

where $\alpha_1, \dots, \alpha_q$ are the roots of $Q(s) = 0$ which we assume to be distinct. It follows that

$$f(t) = \sum_{r=1}^q \frac{1}{Q'(\alpha_r)} e^{\alpha_r t}.$$

Expanding $\exp(\alpha_r t)$ as a Taylor series we have

$$f(t) = \sum_{r=1}^q \frac{1}{Q'(\alpha_r)} \sum_{k=0}^{\infty} \frac{\alpha_r^k t^k}{k!} = \sum_{k=0}^{\infty} \frac{t^k}{k!} \left(\sum_{r=1}^q \frac{\alpha_r^k}{Q'(\alpha_r)} \right).$$

Now, from the theory of residues, we know that if R is sufficiently large so that the circle $\mathcal{C} : |z| = R$ includes all poles of the integrand $z^k/Q(z)$

$$u_k = \sum_{r=1}^q \frac{\alpha_r^k}{Q'(\alpha_r)} = \frac{1}{2\pi i} \oint_{|z|=R} \frac{z^k}{Q(z)} dz.$$

Further, letting $R \rightarrow \infty$ and applying the result

$$\left| \int_{\mathcal{C}} f(z) dz \right| < LM,$$

where L is the length of \mathcal{C} and $M = \max_{\mathcal{C}} |f(z)|$ we find

$$u_k = 0, \quad k = 0, 1, \dots, q-2. \quad (5.3)$$

For $k = q-1$ we make the substitution $z = Re^{i\theta}$ and we find, by letting $R \rightarrow \infty$, that

$$u_{q-1} = 1. \quad (5.4)$$

For larger values of k we can obtain u_k by recursion. This follows from using the fact that if α_r is a root of $Q(s) = 0$

$$u_k = \sum_{r=1}^q \frac{\alpha_r^k}{Q'(\alpha_r)} = - \sum_{r=1}^q \frac{b_1 \alpha_r^{k-1} + b_2 \alpha_r^{k-2} + \cdots + b_q \alpha_r^{k-q}}{Q'(\alpha_r)},$$

or

$$u_k = - \sum_{i=1}^q b_i u_{k-i}, \quad k \geq q. \quad (5.5)$$

Thus we have an expression for $f(t)$,

$$f(t) = \sum_{k=q-1}^{\infty} u_k \frac{t^k}{k!}, \quad (5.6)$$

for which we do not need to find the roots of $Q(s) = 0$. Even when the roots $\alpha_1, \dots, \alpha_q$ are not all distinct as long as the u_k are defined by (5.3), (5.4) and (5.5) the result (5.6) still holds true. We now consider the general case where the numerator $P(s) \neq 1$. We now have

$$f(t) = \sum_{r=1}^q \frac{P(\alpha_r)}{Q'(\alpha_r)} e^{\alpha_r t} = \sum_{k=0}^{\infty} \frac{t^k}{k!} \sum_{r=1}^q \frac{\alpha_r^k P(\alpha_r)}{Q'(\alpha_r)},$$

or

$$f(t) = \sum_{k=0}^{\infty} \frac{v_k t^k}{k!}, \quad (5.7)$$

where

$$v_k = \sum_{r=1}^q \frac{\alpha_r^k P(\alpha_r)}{Q'(\alpha_r)} = \sum_{r=1}^q \frac{\alpha_r^{k+p} + a_1 \alpha_r^{k+p-1} + \cdots + a_p \alpha_r^k}{Q'(\alpha_r)},$$

giving

$$v_k = u_{k+p} + a_1 u_{k+p-1} + \cdots + a_p u_k. \quad (5.8)$$

Equation (5.7) is an expression for $f(t)$ which does not require computation of the roots of $Q(s) = 0$ as the coefficients are obtained recursively from (5.8) and a knowledge of the u_k . Again, this procedure can also be shown to be valid when the roots of $Q(s) = 0$ are repeated. Although, technically, our result is still a sum of exponentials it is effectively a Taylor series expansion and can be evaluated by the methods of Chapter 3.

5.2 The least squares approach to rational Approximation

This approach to determining the Inverse Laplace Transform was advocated by Longman [137] and assumes that we can approximate the function $f(t)$ by $g(t)$,

where

$$g(t) = \sum_1^n A_i e^{-\alpha_i t}. \quad (5.9)$$

Longman seeks to determine the $\{A_i\}$ and $\{\alpha_i\}$, $i = 1, 2, \dots, n$ so that the function S defined by

$$S = \int_0^\infty e^{-wt} [f(t) - g(t)]^2 dt, \quad (5.10)$$

is minimized. $w(\geq 0)$ is a constant and the weight function e^{-wt} is required to ensure convergence of the integral in (5.10). Necessary conditions for S to be a minimum are that

$$\partial S / \partial A_i = 0, \quad \partial S / \partial \alpha_i = 0. \quad (5.11)$$

Since

$$\frac{\partial S}{\partial A_i} = -2 \int_0^\infty e^{-(w+\alpha_i)t} f(t) dt + 2 \sum_{j=1}^n A_j \int_0^\infty e^{-(w+\alpha_i+\alpha_j)t} dt, \quad i = 1, \dots, n$$

the first equation of (5.11) yields

$$\sum_{j=1}^n \frac{A_j}{w + \alpha_i + \alpha_j} = \bar{f}(w + \alpha_i), \quad i = 1, \dots, n. \quad (5.12)$$

Similarly, $\partial S / \partial \alpha_i = 0$ yields

$$\sum_{j=1}^n \frac{A_j}{(w + \alpha_i + \alpha_j)^2} = -\bar{f}'(w + \alpha_i), \quad i = 1, \dots, n. \quad (5.13)$$

In [137] Longman restricts himself to the case where the A_i and α_i are real. He subsequently considered the case where the A_i and α_i occur in complex conjugate pairs (see [142]). To solve the non-linear equations (5.12), (5.13) Longman uses the method of Fletcher-Powell-Davidon [85]. We have found it more convenient to use the method of Gill and Murray [96] as this is available as a NAG Library Routine E04FDF but, whichever method might be used, we have to minimize some real objective function $\phi(x_1, x_2, \dots, x_{2n})$ in $2n$ real variables x_1, x_2, \dots, x_{2n} . In our case we write

$$\begin{aligned} A_1 &= x_1 + ix_2 & \alpha_1 &= x_{n+1} + ix_{n+2} \\ A_2 &= x_1 - ix_2 & \alpha_2 &= x_{n+1} - ix_{n+2} \\ A_3 &= x_3 + ix_4 & \alpha_3 &= x_{n+3} + ix_{n+4} \\ A_4 &= x_3 - ix_4 & \alpha_4 &= x_{n+3} - ix_{n+4} \end{aligned} \quad (5.14)$$

if n is even we terminate with

$$\begin{aligned} A_{n-1} &= x_{n-1} + ix_n & \alpha_{n-1} &= x_{2n-1} + ix_{2n} \\ A_n &= x_{n-1} - ix_n & \alpha_n &= x_{2n-1} - ix_{2n} \end{aligned} \quad (5.14a)$$

while if n is odd we end with

$$A_n = x_n \quad \alpha_n = x_{2n}. \quad (5.14b)$$

The function ϕ we can take as

$$\begin{aligned} \phi = \sum_{i=1}^n \left[\left| \sum_{j=1}^n \frac{A_j}{w + \alpha_i + \alpha_j} - \bar{f}(w + \alpha_i) \right|^2 \right. \\ \left. + \left| \sum_{j=1}^n \frac{A_j}{(w + \alpha_i + \alpha_j)^2} + \bar{f}'(w + \alpha_i) \right|^2 \right], \end{aligned} \quad (5.15)$$

and we consider the equations (5.12), (5.13) to be solved if, given some small prescribed ϵ , we can find x_1, x_2, \dots, x_{2n} such that

$$\phi < \epsilon.$$

Note that the minimization procedure might give us a local minimum of ϕ (or S) so that it will be necessary to compare the results associated with several trial values for the vector $\mathbf{x} = (x_1, \dots, x_{2n})$ before we arrive at an absolute minimum.

Because of the geometry of the objective function local minima abound and one has to be very shrewd in ones acceptance of results. While one would expect more accurate approximation by exponential sums as n increases, and Sidi [211] has established this property, the proliferation of local minima makes it a difficult task to realise.

5.2.1 Sidi's Window Function

Sidi [212] extended the approach of Longman by replacing the weight function e^{-wt} by a 'window' function $\Psi(t)$. Sidi's rationale in introducing this function was that for small values of t the function $g(t)$ would approximate $f(t)$ closely but because of the strong damping effect of $\exp(-wt)$ there could be a substantial deviation between $g(t)$ and $f(t)$ for larger t . However,

$$\Psi(t) = t^N e^{-wt}, \quad (5.16)$$

where N is a positive integer and $w > 0$ has the property of having a maximum, call it Ψ_0 , at $t = N/w$ and being greater than $\frac{1}{2}\Psi_0$ in an interval of $2\sqrt{N}/w$ on either side of the maximum before tailing off to zero at $t = 0$ on the left and some multiple of N on the right. The net effect of the weight function $\Psi(t)$ is to ensure a good approximation to $f(t)$ in the window $[N - \sqrt{N}/w, N + \sqrt{N}/w]$. Note that the choice of $\Psi(t)$ is restricted by the requirement that

$$\int_0^\infty \Psi(t)f(t)dt,$$

needs to be expressed as a simple function of $\bar{f}(s)$.

With $g(t)$ defined as before in (5.9) and defining S' by

$$S' = \int_0^\infty \Psi(t)(f(t) - g(t))^2 dt, \quad (5.17)$$

we have

$$\begin{aligned} S' &= \int_0^\infty \Psi(t)[f(t)]^2 dt - 2 \sum_{i=1}^n A_i \int_0^\infty \Psi(t) e^{-\alpha_i t} f(t) dt \\ &\quad + \sum_{i=1}^n \sum_{j=1}^n A_i A_j \int_0^\infty \Psi(t) e^{-\alpha_i t} e^{-\alpha_j t} dt, \end{aligned}$$

which reduces to

$$\begin{aligned} S' &= \int_0^\infty \Psi(t)[f(t)]^2 dt - 2 \sum_{i=1}^n A_i (-1)^N \bar{f}^{(N)}(\alpha_i + w) \\ &\quad + \sum_{i=1}^n \sum_{j=1}^n A_i A_j N! / (\alpha_i + \alpha_j + w)^{N+1}. \end{aligned} \quad (5.18)$$

The best approximation in the least squares sense is the one which satisfies

$$\partial S' / \partial A_i = 0, \quad \partial S' / \partial \alpha_i = 0, \quad (5.19)$$

that is

$$\bar{g}^{(N)}(\alpha_i + w) = \bar{f}^{(N)}(\alpha_i + w), \quad i = 1, \dots, n, \quad (5.20)$$

$$\bar{g}^{(N+1)}(\alpha_i + w) = \bar{f}^{(N+1)}(\alpha_i + w), \quad i = 1, \dots, n. \quad (5.21)$$

The techniques for solving non-linear equations mentioned previously can now be brought into play to determine the A_i and α_i .

5.2.2 The Cohen-Levin Window Function

Ideally, a pulse function such as $H(t - a) - H(t - b)$, $a < b$ would be the preferred choice for $\Psi(t)$ as only behaviour in the interval (a, b) would be minimised and anything extraneous would be ignored. This has to be ruled out as it does not enable us to express the integral in (5.17) in terms of a simple function of $\bar{f}(s)$. Since $x = e^{-wt}$ only varies between 0 and 1 for $t \in [0, \infty)$, $w > 0$, the question that can be asked is:- Can we find a polynomial $p(x)$ which is large in the window region $[d, 1 - d]$ but which is small outside or, more precisely, which satisfies

$$\begin{aligned} |p(x)| &< m (< 1) \quad x \in [0, d], [1 - d, 1] \\ |p(x)| &> m \quad d \leq x \leq 1 - d, \end{aligned}$$

and

$$|p(\frac{1}{2})| = 1?$$

The answer is in the affirmative. It is well-known that the Chebyshev polynomial $T_n(x)$ is equi-oscillatory in $[-1, 1]$ and increases unboundedly outside that interval. Thus we can construct $p(x)$ by choosing it to be symmetric about $x = \frac{1}{2}$ and to have equi-oscillatory behaviour in $[0, d]$. The required polynomial is

$$p(x) = \frac{T_n\left(\frac{(2x-1)^2 - \frac{1}{2}(1+D)}{\frac{1}{2}(1-D)}\right)}{T_n\left(\frac{-\frac{1}{2}(1+D)}{\frac{1}{2}(1-D)}\right)},$$

where $D = (1 - 2d)^2$. Since the window function has to be positive $p(x)$ cannot fulfil this role but $[p(x)]^2$ can and thus we choose

$$\Psi(t) = [p(x)]^2, \quad x = e^{-wt}. \quad (5.22)$$

The simplest case is when $n = 2$. If we take $d = 0.25$, for example, then

$$\begin{aligned} p(x) &\propto [T_2(\frac{8}{3}\{(2x-1)^2 - \frac{5}{8}\})]^2, \\ &\propto 32x^4 - 64x^3 + 38x^2 - 6x + \frac{9}{64}, \end{aligned}$$

yielding

$$\begin{aligned} [p(x)]^2 &= 1024x^8 - 4096x^7 + 6528x^6 - 5248x^5 + 2221x^4 \\ &\quad - 474x^3 + 46\frac{11}{16}x^2 - 1\frac{11}{16}x + \frac{81}{4096}. \end{aligned}$$

There is still a drawback about having (5.22) as a window function namely the presence of the constant term in $[p(x)]^2$ as convergence of the integral (5.17) cannot now be guaranteed. This can be resolved to some extent by taking

$$\Psi(t) = x[p(x)]^2, \quad x = e^{-wt}. \quad (5.23)$$

We mention that for general d , $0 < d < 0.5$ and $n = 2$ we have

$$p(x) = 32x^4 - 64x^3 + (40 - 8D)x^2 - 8(1 - D)x + \frac{1}{4}(1 - D)^2.$$

$\Psi(t)$ can be evaluated from (5.22). We can similarly establish window functions corresponding to $n = 3, 4$, etc.

A further improvement to the above method can be made by multiplying $\Psi(t)$ by the Sidi window function. If we arrange for the maximum of the Sidi window function to coincide with the maximum of $\Psi(t)$ then the product of the two functions will reinforce the contribution to the least squares integral in the window interval and decrease the contribution outside.¹

¹The author wishes to thank the Royal Society for supporting the above research by contributing to a travel grant.

5.3 Padé, Padé-type and Continued Fraction Approximations

One approach to obtaining rational approximations to a given Laplace transform is to determine a continued fraction approximation to the transform. Thus, for example, if $\bar{f}(s) = e^{-1/s}g(s)$, where $g(s)$ is a rational function of s , we could determine a continued fraction approximation for $e^{-1/s}$ by the method of Thiele (§11.5), curtail it at some appropriate convergent, and then multiply it by $g(s)$ and apply the results of §5.1. This is illustrated by the following example:

Example 5.2 Determine a continued fraction expansion for $f(x) = e^{-x}$. Hence find a rational approximation for $e^{-1/s}/s$.

We have, following §11.5, $\rho_{-2}(x) = \rho_{-1}(x) = 0$, $\phi_0(x) = e^{-x}$. From (11.78)

$$\rho_0(x) = e^{-x},$$

and from (11.79)

$$\phi_1(x) = 1/(-e^{-x}) = -e^x.$$

Similarly we find

$$\begin{aligned}\rho_1(x) &= -e^x, & \phi_2(x) &= -2e^{-x}, \\ \rho_2(x) &= -e^{-x}, & \phi_3(x) &= 3e^x,\end{aligned}$$

and, in general, we obtain by induction that

$$\begin{aligned}\phi_{2r}(x) &= (-1)^r 2e^{-x}, & \phi_{2r+1}(x) &= (-1)^{r+1} (2r+1)e^x, \\ \rho_{2r}(x) &= (-1)^r e^{-x}, & \rho_{2r+1}(x) &= (-1)^{r+1} (r+1)e^x.\end{aligned}$$

Thus the continued fraction expansion about $x = 0$ is

$$e^{-x} = 1 + \frac{x}{-1+} \frac{x}{-2+} \frac{x}{3+} \frac{x}{2+} \frac{x}{-5+} \frac{x}{-2+\dots}.$$

Curtailling this at the term $x/3$ we find

$$e^{-x} \approx \frac{1 - \frac{2}{3}x + \frac{1}{6}x^2}{1 + \frac{1}{3}x}.$$

It follows that

$$\frac{e^{-1/s}}{s} \approx \frac{s^2 - \frac{2}{3}s + \frac{1}{6}}{s^2(s + \frac{1}{3})}.$$

Since the Laplace transform of the right hand side is

$$\frac{9}{2}e^{-t/3} + \frac{1}{2}t - \frac{7}{2}$$

we have an approximation to the inverse transform. When $t = 1$ the approximation gives $f(t) \approx 0.22439$. The exact inverse transform is, from §11.1, $J_0(2\sqrt{t})$ and, when $t = 1$ this has the value 0.22389. We would expect to get better results by taking more terms in the continued fraction expansion. Note, however, that with the above approximation we cannot expect good results for large t as $f(t) \sim t/2$ whereas

$$J_0(2\sqrt{t}) \rightarrow 0 \quad \text{as} \quad t \rightarrow \infty.$$

Luke [148], [147] and [149] has suggested that when $\bar{f}(s)$ is a complicated function of s then $\bar{f}(s)$ should be approximated by a sequence of rational functions $\bar{f}_n(s)$ the inverses of which, hopefully, will rapidly converge to $f(t)$ as $t \rightarrow \infty$ in some interval $0 \leq t \leq T$ or, alternatively, for $t \geq T$ where T is specified.

Longman [137] has used the method of Padé approximants to find rational approximations for the inverse Laplace transform and illustrates the method with the example

$$\bar{f}(s) = (1/s) \exp\{-s/(1 + \sigma s)^{1/2}\}, \quad \sigma > 0 \quad (5.24)$$

First he finds the Maclaurin expansion of $s\bar{f}(s)$ which is

$$s\bar{f}(s) = \sum_{k=0}^{\infty} a_k s^k, \quad (5.25)$$

where

$$a_0 = 1, \quad a_1 = -1, \quad a_2 = (1 + \sigma)/2,$$

and

$$a_k = (-1)^k \left\{ \frac{1}{k!} + \frac{\sigma/2}{(k-2)!} + \sum_{r=2}^{k-1} \frac{(k-r+2)(k-r+4) \cdots (k+r-2)}{(k-r-1)!r!} \left(\frac{\sigma}{2}\right)^r \right\}, \quad k > 2. \quad (5.26)$$

In the special case where $\sigma = 0$ we have $\bar{f}(s) = e^{-s}/s$ giving $f(t) = H(t-1)$. Also if s is sufficiently large $\bar{f}(s) \approx g(s) = (1/s) \exp\{-(s/\sigma)^{1/2}\}$ so that for very small t we can expect $f(t) \approx g(t) = \operatorname{erfc}[\frac{1}{2}(\sigma t)^{-1/2}]$.

We now have to find the Padé approximants. Longman [136] has given simple recursion formulae for computing the coefficients in the Padé table, which is assumed normal, and avoids the evaluation of determinants of high order. Suppose

$$E_{pq} = P(s)/Q(s), \quad (5.27)$$

is the $[p/q]$ Padé approximant (see Appendix 11.5 for notation adopted) of $s\bar{f}(s)$ where we fix c_0 to be 1. Then the $[p-1, q]$ and $[p, q-1]$ approximants satisfy

$$(a_0 + a_1 s + \cdots)(\gamma_0 + \gamma_1 s + \cdots + \gamma_q s^q) = \beta_0 + \beta_1 s + \cdots + \beta_{p-1} s^{p-1} + 0s^p + \cdots + 0s^{p+q-1} + O(s^{p+q}), \quad (5.28)$$

and

$$(a_0 + a_1s + \cdots)(\gamma'_0 + \gamma'_1s + \cdots + \gamma'_{q-1}s^{q-1}) = \beta'_0 + \beta'_1s + \cdots + \beta'_ps^p + 0s^{p+1} + \cdots + 0s^{p+q-1} + O(s^{p+q}). \quad (5.29)$$

Subtracting (5.29) from (5.28) we have on noting that $\gamma_0 = \gamma'_0 = 1$ and $\beta_0 = \beta'_0 = a_0$ and simplifying

$$\begin{aligned} & (a_0 + a_1s + \cdots)[(\gamma_1 - \gamma'_1) + (\gamma_2 - \gamma'_2)s + \cdots + (\gamma_{q-1} - \gamma'_{q-1})s^{q-2} + \gamma_qs^{q-1}] \\ &= (\beta_1 - \beta'_1) + (\beta_2 - \beta'_2)s + \cdots + (\beta_{p-1} - \beta'_{p-1})s^{p-2} - \beta'_ps^{p-1} \\ &+ 0s^p + 0s^{p+1} + \cdots + 0s^{p+q-2} + O(s^{p+q-1}). \end{aligned} \quad (5.30)$$

If $\gamma_1 - \gamma'_1 = 1$ the above equation would represent the $[p-1, q-1]$ approximant. However, this is not generally the case and we have to divide both sides of (5.30) by $\gamma_1 - \gamma'_1$ (which cannot vanish in a normal table) to determine the $[p-1, q-1]$ approximant. Calling the coefficients in the numerator B_i , $i = 0, \dots, p-1$ and those in the denominator Γ_i , $i = 0, \dots, q-1$ we see that

$$\begin{aligned} \Gamma_i &= \frac{\gamma_{i+1} - \gamma'_{i+1}}{\gamma_1 - \gamma'_1}, \quad i = 1, \dots, q-2 \\ \Gamma_{q-1} &= \frac{\gamma_q}{\gamma_1 - \gamma'_1}, \end{aligned} \quad (5.31)$$

and

$$\begin{aligned} B_{i-1} &= \frac{\beta_i - \beta'_i}{\gamma_1 - \gamma'_1}, \quad i = 1, \dots, p-1 \\ B_{p-1} &= -\frac{\beta'_p}{\gamma_1 - \gamma'_1}. \end{aligned} \quad (5.32)$$

Clearly $B_0 = a_0$ and Γ_0 is by construction equal to 1. The relations (5.32) can also be written as

$$\begin{aligned} B_0 &= a_0, \quad B_{i-1} = a_0 \frac{\beta_i - \beta'_i}{\beta_1 - \beta'_1}, \quad i = 2, \dots, p-1 \\ B_{p-1} &= -a_0 \frac{\beta'_p}{\beta_1 - \beta'_1}. \end{aligned} \quad (5.33)$$

The recurrence relations (5.31) and (5.33) can be used to build up the Padé table starting from the first row and column in the following way. We have

$$\left. \begin{aligned} \gamma'_0 &= 1 \\ \gamma'_i &= \gamma_i - \frac{\Gamma_{i-1}\gamma_q}{\Gamma_{q-1}} \end{aligned} \right\} \quad i = 1, 2, \dots, q-1 \quad (5.34)$$

and

$$\left. \begin{aligned} \beta_0 &= a_0 \\ \beta_i &= \beta'_i - \frac{B_{i-1}\beta'_p}{B_{p-1}} \quad i = 1, 2, \dots, p-1 \end{aligned} \right\} \quad (5.35)$$

Now E_{p0} is just

$$a_0 + a_1 s + \dots + c_p s^p,$$

and thus given the first $n+1$ coefficients a_0, a_1, \dots, a_n of $\bar{f}(s)$ we can compute the coefficients E_{ij} , $i+j \leq n$ in the triangle

$$\begin{array}{cccccc} E_{00} & E_{01} & E_{02} & E_{03} & \cdots & E_{0n} \\ E_{10} & E_{11} & E_{12} & \cdots & E_{1,n-1} & \\ E_{20} & E_{21} & \cdots & E_{2,n-2} & & \\ E_{30} & \cdots & & & & \\ \vdots & & & & & \\ E_{n0} & & & & & \end{array} \quad (5.36)$$

from a knowledge of $E_{00}, E_{01}, \dots, E_{0n}$, which can be computed from

$$\left. \begin{aligned} \gamma_0 &= 1 \\ \gamma_1 &= -a_1/a_0 \\ \gamma_2 &= -(a_2 + a_1\gamma_1)/a_0 \\ \dots\dots\dots \\ \gamma_n &= -(a_n + a_{n-1}\gamma_1 + \dots + a_1\gamma_{n-1})/a_0 \end{aligned} \right\} \quad (5.37)$$

and

$$\beta_0 = a_0.$$

For the function defined by (5.24) we have used the program LONGPAD, which can be downloaded from the URL

www.cf.ac.uk/maths/cohen/programs/inverselaplace transform/ ,

to determine the diagonal elements in the Padé Table for $s\bar{f}(s)$ and we obtained the results in Table 5.1 when $\sigma = 1$.

The approximations to $\bar{f}(s)$ are then $\bar{f}_n(s) = E_{nn}/s$ giving a corresponding approximation $f_n(t)$ to $f(t)$. Thus we have, for example,

$$f_2(t) = 1 - e^{-2.73764t}(0.45627 \cos bt + 6.16775 \sin bt), \quad b = 1.27702;$$

$$\begin{aligned} f_4(t) &= 1 + e^{a_1 t}(3.262493 \cos b_1 t - 60.32278 \sin b_1 t) \\ &\quad + e^{a_2 t}(-4.143798 \cos b_2 t + 14.536713 \sin b_2 t), \end{aligned}$$

where

$$\begin{aligned} a_1 &= -4.624887 & b_1 &= 0.950494 \\ a_2 &= -4.633295 & b_2 &= 3.322285 . \end{aligned}$$

These approximations give exactly the same results as those found by Longman [137]. See, however, Longman [140] where an alternative approach is adopted.

k	E_{kk}
2	$\frac{1-0.4s+0.0595833s^2}{1+0.6s+0.1095833s^2}$
3	$\frac{1-0.35s+0.0552443s^2-0.004068s^3}{1+0.65s+0.1552443s^2+0.0140927s^3}$
4	$\frac{1-0.3s+0.0439073s^2-0.0037713s^3+0.0001638s^4}{1+0.7s+0.1939073s^2+0.0255527s^3+0.0013800s^4}$
5	$\frac{1-0.25s+0.0318916s^2-0.0026204s^3+0.0001401s^4-0.0000039s^5}{1+0.75s+0.2318916s^2+0.03718790s^3+0.0031209s^4+0.0001111s^5}$

Table 5.1: Padé table for $s\bar{f}(s)$, $\bar{f}(s)$ defined by (5.24).

Van Iseghem [242] developed an interesting method for inverting Laplace transforms using Padé-type approximants. She assumes that the function $f(t)$ can be expressed in the form

$$f(t) = e^{-\lambda t} \sum_{n \geq 0} a_n L_n(2\lambda t), \quad (5.38)$$

where L_n denotes the Laguerre polynomial of degree n . It follows that

$$\bar{f}(s) = \frac{1}{s + \lambda} \sum_{n \geq 0} a_n \left(\frac{s - \lambda}{s + \lambda} \right)^n. \quad (5.39)$$

If $\bar{f}_m(s)$ denotes the m -th partial sum of (5.39) it can be considered as a $(m/m+1)$ Padé-type approximant of \bar{f} with denominator $(s + \lambda)^{m+1}$ and, at the point $s = \lambda$, \bar{f} has a Taylor series expansion

$$\bar{f}(s) = \sum_{n \geq 0} c_n (s - \lambda)^n, \quad \text{such that} \quad \bar{f}(s) - \bar{f}_m(s) = O((s - \lambda)^{m+1}). \quad (5.40)$$

Van Iseghem shows that the coefficients a_n can be determined from the equation

$$a_n = \sum_{i=0}^n \binom{n}{i} c_i (2\lambda)^{i+1}, \quad (5.41)$$

which enables the terms in (5.38) to be computed. Various theoretical convergence properties are established but crucial to the whole method is the choice of λ as there could be severe cancellation arising in the computation of (5.41) because of the binomial coefficients coupled with the fact that λ can be greater than 1. She makes improvements to the method, firstly by a choice of λ which leads to the best rate of convergence of the series (5.39), secondly by a modification that leads to convergence of the series in the least square sense by

using as a weight function the Sidi window function. Full details of the method can be found in van Iseghem's paper [242]. Expansions in terms of Laguerre polynomials have been determined by other methods in Chapter 3.

5.3.1 Prony's method and z-transforms

If a function $f(t)$ is given by

$$f(t) = \sum_{j=1}^n A_j e^{b_j t}, \quad (5.42)$$

and $f(t)$ is known at the $2n$ ordinates kT , $k = 0, 1, \dots, 2n-1$ then the $2n$ parameters A_j , b_j , $j = 1, 2, \dots, n$ can be determined by a method due originally to Prony [65]. Weiss and McDonough [249] determine the unknown parameters in the following way. Since $f(kT) = f_k$ is known for $k = 0, 1, \dots, 2n-1$ its z-transform has the form

$$F(z) = f_0 + f_1 z^{-1} + \dots + f_{2n-1} z^{-(2n-1)} + \dots \quad (5.43)$$

Now

$$\mathcal{Z}\{e^{b_j T}\} = \frac{z}{z - e^{b_j T}} = \frac{z}{z - z_j},$$

where $z_j = \exp(b_j T)$ and thus

$$\begin{aligned} \mathcal{Z}\left\{\sum_{j=1}^n A_j e^{b_j T}\right\} &= \sum_{j=1}^n \frac{A_j z}{z - z_j} \\ &= \frac{a_n z^n + a_{n-1} z^{n-1} + \dots + a_1 z}{z^n + \alpha_{n-1} z^{n-1} + \dots + \alpha_1 z + \alpha_0} \end{aligned} \quad (5.44)$$

where the denominator is $\prod_{j=1}^n (z - z_j)$.

Equating (5.43) and (5.44) and rearranging we see that we have the classical Padé formulation

$$\begin{aligned} a_n z^n + a_{n-1} z^{n-1} + \dots + a_1 z &= (z^n + \alpha_{n-1} z^{n-1} + \dots + \alpha_1 z + \alpha_0) \cdot \\ &\quad \cdot (f_0 + f_1 z^{-1} + \dots + f_{2n-1} z^{-(2n-1)} + \dots). \end{aligned}$$

Equating like powers of z yields

$$\left. \begin{aligned} f_0 &= a_n \\ f_0 \alpha_{n-1} + f_1 &= a_{n-1} \\ \vdots & \\ f_0 \alpha_1 + f_1 \alpha_2 + \dots + f_{n-2} \alpha_{n-1} + f_{n-1} &= 0 \end{aligned} \right] \quad (5.45)$$

and

$$\left. \begin{aligned} f_0 \alpha_0 + f_1 \alpha_1 + \dots + f_{n-1} \alpha_{n-1} + f_n &= 0 \\ f_1 \alpha_0 + f_2 \alpha_1 + \dots + f_n \alpha_{n-1} + f_{n+1} &= 0 \\ \vdots & \\ f_{n-1} \alpha_0 + f_n \alpha_1 + \dots + f_{2n-2} \alpha_{n-1} + f_{2n-1} &= 0 \end{aligned} \right] \quad (5.46)$$

Solution of the linear equations (5.46) enables the α_j to be determined and, by finding the eigenvalues of the companion matrix (§11.7) we can determine the z_j which are the roots of the polynomial equation

$$z^n + \alpha_{n-1}z^{n-1} + \cdots + \alpha_1z + \alpha_0 = 0.$$

The parameters b_j are then immediately determined from the equation

$$b_j = \frac{1}{T} \ln z_j. \quad (5.47)$$

Finally, the $\{a_j\}$ can be computed from (5.45) and this enables us to compute the $\{A_j\}$ as they are the numerators in the partial fraction expansion

$$\frac{1}{z}F(z) = \sum_{j=1}^n \frac{A_j}{z - z_j}. \quad (5.48)$$

We give an example to illustrate the method.

Example 5.3 If it is known that

$$f(t) = A_1e^{b_1t} + A_2e^{b_2t} + A_3e^{b_3t},$$

determine A_1, A_2, A_3 and b_1, b_2, b_3 given the data

$$f_0 = 2.5, f_1 = 0.58731, f_2 = 0.22460, f_3 = 0.08865, f_4 = 0.03416, f_5 = 0.01292,$$

where $f_n = f(nT)$ and $T = 1$. Solution of the equations (5.46) yields

$$\alpha_2 = -0.6424221998, \quad \alpha_1 = 0.1122057146, \quad \alpha_0 = -0.004104604860.$$

Substitution in (5.45) gives

$$a_3 = 2.5, \quad a_2 = -1.0187454995, \quad a_1 = 0.12781330433.$$

The quantities z_j are the roots of the cubic equation

$$z^3 - 0.6424221998z^2 + 0.1122057146z - 0.004104604860 = 0,$$

and are found to be

$$z_1 = 0.3674771169, \quad z_2 = 0.02253873364, \quad z_3 = 0.04955774567.$$

Since $T = 1$ it follows from (5.47) that

$$b_1 = -1.0010942292, \quad b_2 = -1.4899348617, \quad b_3 = -3.0046167110.$$

Finally we have

$$\begin{aligned} \frac{1}{z}F(z) &= \frac{2.5z^2 - 1.0187454995z + 0.12781330433}{(z - z_1)(z - z_2)(z - z_3)}, \\ &= \frac{2.015496762}{z - z_1} - \frac{1.008646087}{z - z_2} + \frac{1.493149325}{z - z_3}. \end{aligned}$$

The data was generated by rounding the values of $f(t) = 2e^{-t} - e^{-1.5t} + 1.5e^{-3t}$ at $t = 0, 1, \dots, 5$ to 5 decimal places. Clearly, the error in the data caused by rounding has led to a perturbation in the coefficients of the polynomial in z which has affected the roots and the subsequent determination of the A_j . The reader should repeat the analysis with data rounded to 3 decimal places.

5.3.2 The Method of Grundy

The methods of earlier sections and Padé approximants effectively enable us to compute the function $f(t)$ in a region around $t = 0$ for positive values of t . These approximations are usually poor for large values of t . Grundy [108] tackles this problem by constructing two point rational approximants in the form of continued fractions.

Suppose that a function $g(z)$ can be expanded about $z = 0$ in the series

$$g(z) = \sum_{n=0}^{\infty} c_n z^n \quad (5.49)$$

and about $z = \infty$ in the form

$$g(z) = \sum_{n=1}^{\infty} b_n z^{-n} \quad (5.50)$$

(5.49) and (5.50) may be either convergent or asymptotic. The leading coefficients c_0 and b_1 must be non-zero but other coefficients may be zero. The object of the Grundy method is to construct a continued fraction, called a M -fraction, which has the form

$$M_m(z) = \frac{c_0}{1 + d_1 z} + \frac{n_2 z}{1 + d_2 z} + \dots + \frac{n_m z}{1 + d_m z}, \quad (5.51)$$

which has the property that it agrees with m terms of (5.49) and m terms of (5.50).

In some applications the above might not be possible and the best that can be achieved is the construction of a continued fraction $M_{p,q}(z)$ which fits $p + q$ terms of (5.49) and $p - q$ terms of (5.50). In the case where $p = m + r$ and $q = r$ we have

$$M_{m+r,r}(z) = \frac{c_0}{1 + d_1 z} + \frac{n_2 z}{1 + d_2 z} + \dots + \frac{n_m z}{1 + d_m z} + \frac{n_{m+1} z}{1} + \frac{n_{m+2} z}{1} + \dots + \frac{n_{m+2r} z}{1} \quad (5.52)$$

Since we know from Chapter 2, (2.40)-(2.43), that under certain conditions the Laplace transform $\tilde{f}(s)$ can be expanded as either a convergent series in $1/s$ for $|s| > R$ or as a power series we can, in these cases, write down directly expansions for $f(t)$. Grundy gives the example

$$\tilde{f}(s) = \frac{1}{\sqrt{s}(\sqrt{s} + a)}, \quad (5.53)$$

t	M_3	M_5	M_7	Exact
1.0	0.426858	0.427578	0.427584	0.427584
2.0	0.335538	0.336198	0.336204	0.336204
3.0	0.286774	0.287337	0.287341	0.287341
4.0	0.254913	0.255390	0.255396	0.255396
5.0	0.231913	0.232321	0.232326	0.232326

Table 5.2: Convergents to $f(t)$ in Grundy's method when $\bar{f}(s) = 1/\sqrt{s}(\sqrt{s+1})$. (Reproduced from [108] with permission)

where

$$\bar{f}(s) = \frac{1}{s} \sum_{n=0}^{\infty} (-1)^n \left(\frac{a}{s^{1/2}} \right)^n, \quad |s| > a^2, \quad (5.54)$$

and consequently

$$f(t) = \sum_{n=0}^{\infty} \frac{(-1)^n a^n t^{n/2}}{\Gamma(1 + \frac{n}{2})}. \quad (5.55)$$

Again we can show that

$$\bar{f}(s) = \frac{1}{a\sqrt{s}} \sum_{n=0}^{\infty} (-1)^n \left(\frac{\sqrt{s}}{a} \right)^n, \quad |s| < a^2, \quad (5.56)$$

which yields the asymptotic expansion for $f(t)$ as $t \rightarrow \infty$

$$f(t) \sim \sum_{n=0}^{\infty} \frac{(-1)^n t^{-(n+1)/2}}{a^{n+1} \Gamma(\frac{1-n}{2})}. \quad (5.57)$$

If we put $t = z^2$ in (5.55) and (5.57) then we have series of the form (5.49) and (5.50) respectively and the M -fractions can be computed by a method due to McCabe and Murphy [152]. With $a = 1$ Grundy constructed Table 5.2. Note that the exact answer is

$$f(t) = e^{a^2 t} \operatorname{erfc}(a\sqrt{t}). \quad (5.58)$$

5.4 Multidimensional Laplace Transforms

Singhal et al [221] have given a method for the numerical inversion of two dimensional Laplace transforms which can be extended to higher dimensions. The method is based on the method of Padé approximation. From the inversion formula we have

$$f(t_1, t_2) = \left(\frac{1}{2\pi i} \right) \int_{c_1 - i\infty}^{c_1 + i\infty} \int_{c_2 - i\infty}^{c_2 + i\infty} \bar{f}(s_1, s_2) e^{s_1 t_1} e^{s_2 t_2} ds_1 ds_2 \quad (5.59)$$

By making the substitution

$$s_k t_k = z_k, \quad k = 1, 2$$

(5.59) becomes

$$f(t_1, t_2) = \frac{1}{t_1 t_2} \left(\frac{1}{2\pi i} \right) \int_{c'_1 - i\infty}^{c'_1 + i\infty} \int_{c'_2 - i\infty}^{c'_2 + i\infty} \bar{f} \left(\frac{z_1}{t_1}, \frac{z_2}{t_2} \right) e^{z_1} e^{z_2} dz_1 dz_2. \quad (5.59')$$

Now

$$e^{z_k} \approx [N_k/M_k](z_k) = \frac{\sum_{i=0}^{N_k} (M_k + N_k - i)! \binom{N_k}{i} z_k^i}{\sum_{i=0}^{M_k} (-1)^i (M_k + N_k - i)! \binom{M_k}{i} z_k^i}, \quad k = 1, 2$$

where $N_k < M_k$. We can write the right hand side in the form

$$[N_k/M_k](z_k) = \sum_{i=1}^{M_k} \frac{R_{ki}}{z_k - z_{ki}}$$

where z_{ki} are the poles of the approximation (assumed distinct) and R_{ki} are the corresponding residues. Substituting $[N_k/M_k](z_k)$ for e^{z_k} in (5.59') we obtain

$$\begin{aligned} \tilde{f}(t_1, t_2) = & \frac{1}{t_1 t_2} \left(\frac{1}{2\pi i} \right)^2 \int_{c'_1 - i\infty}^{c'_1 + i\infty} \int_{c'_2 - i\infty}^{c'_2 + i\infty} \bar{f} \left(\frac{z_1}{t_1}, \frac{z_2}{t_2} \right) \\ & \cdot \sum_{i=1}^{M_1} \frac{R_{1i}}{z_1 - z_{1i}} \sum_{i=1}^{M_2} \frac{R_{2i}}{z_2 - z_{2i}} dz_1 dz_2 \end{aligned}$$

where \tilde{f} is an approximation to f . If summation and integration are interchanged in the above we find

$$\begin{aligned} \tilde{f}(t_1, t_2) = & \frac{1}{t_1 t_2} \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \left\{ R_{1j} R_{2k} \left(\frac{1}{2\pi i} \right)^2 \right. \\ & \cdot \left. \int_{c'_1 - i\infty}^{c'_1 + i\infty} \int_{c'_2 - i\infty}^{c'_2 + i\infty} \frac{\bar{f}(z_1/t_1, z_2/t_2)}{(z_1 - z_{1j})(z_2 - z_{2k})} dz_1 dz_2 \right\} \end{aligned}$$

On the assumption that \bar{f} has no poles within an appropriate contour application of the calculus of residues yields

$$\tilde{f}(t_1, t_2) = \frac{1}{t_1 t_2} \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} R_{1j} R_{2k} \bar{f} \left(\frac{z_{1j}}{t_1}, \frac{z_{2k}}{t_2} \right). \quad (5.60)$$

Singhal et al note that functions of the form

$$\bar{f}(s_1, s_2) = \frac{1}{s_1^{m_1} s_2^{m_2}}$$

are inverted exactly if $m_1 \leq M_1 + N_1 + 1$ and $m_2 \leq M_2 + N_2 + 1$. and consequently their method will work well for functions which are well-approximated by truncated Taylor series.

Chapter 6

The Method of Talbot

6.1 Early Formulation

This method is based on the evaluation of the inversion integral

$$f(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \bar{f}(s) ds, \quad t > 0. \quad (6.1)$$

where c is real and $c > \gamma$, which ensures that all singularities are to the left of the line $\Re s = c$. Direct numerical evaluation of the right hand side of (6.1) has to take account of the oscillations of e^{st} as $\Im s \rightarrow \pm\infty$. Talbot's method overcomes this difficulty by avoiding it. The line $\mathfrak{B} : (c-i\infty, c+i\infty)$ is replaced by an equivalent contour \mathfrak{B}' starting and ending in the left half-plane so that $\Re s \rightarrow -\infty$ at each end. This replacement is permissible if

- (i) \mathfrak{B}' encloses all singularities of $\bar{f}(s)$;

and

- (ii) $|\bar{f}(s)| \rightarrow 0$ uniformly in $\Re s \leq \gamma$ as $|s| \rightarrow \infty$.

Condition (ii) holds for almost all functions likely to be encountered except for those with an infinity of singularities on the imaginary axis. Condition (i) may not be satisfied by a given $\bar{f}(s)$ with a particular \mathfrak{B}' , but can generally be made to hold for the modified function $f(\lambda s + \sigma)$ by suitable choice of the scaling parameter λ and the shift parameter σ . Thus, if $\bar{f}(s)$ has a singularity s_0 , $\bar{f}(\lambda s + \sigma)$ has a corresponding singularity s_0^* given by

$$s_0^* = (s_0 - \sigma)/\lambda, \quad (6.2)$$

and (6.1) can be replaced by

$$f(t) = \frac{\lambda e^{\sigma t}}{2\pi i} \int_{\mathfrak{B}'} e^{\lambda s t} \bar{f}(\lambda s + \sigma) ds, \quad t > 0 \quad (6.3)$$

In the first version of the method (Talbot [226]), based on a thesis by Green [106], the contour \mathfrak{B}' was taken to be a steepest descent contour through a saddle-point of the integral $\int e^{w(s)} ds$, i.e. a zero of $dw/ds, w = u + iv$. This would be quite impractical to work out for each function $\bar{f}(s)$ to be inverted but Talbot reasoned that the steepest descent contour for any $\bar{f}(s)$ is likely to produce good results for all $\bar{f}(s)$ and therefore took the steepest descent contour for $\bar{f}(s) = 1/s$. This choice of $\bar{f}(s)$ gives

$$w(s) = s - \ln s,$$

and the saddle point is $\hat{s} = 1, \hat{v} = 0$. The steepest descent contour is, taking $\theta = \arg s$ as a parameter,

$$\mathfrak{B}' : s = \alpha + i\theta, \quad \alpha = \theta \cot \theta, \quad -\pi < \theta < \pi. \quad (6.4)$$

(6.3) becomes in terms of θ

$$f(t) = \frac{\lambda e^{\sigma t}}{2\pi i} \int_{\mathfrak{B}'} e^{\lambda s t} \bar{f}(\lambda s + \sigma) \frac{ds}{d\theta} d\theta. \quad (6.5)$$

As θ varies between $-\pi$ and π we can apply the trapezium rule for integration to approximate $f(t)$. Call the approximation $\tilde{f}(t)$. Then

$$\tilde{f}(t) = \frac{\lambda e^{\sigma t}}{2\pi i} \cdot \frac{\pi}{n} \sum_{-n}^n \left[e^{\lambda t(\alpha_k + i\theta_k)} \bar{f}(\lambda(\alpha_k + i\theta_k) + \sigma) \right] (\cot \theta - \theta \csc^2 \theta + i)_{\theta=\theta_k}, \quad (6.6)$$

where $\theta_k = k\pi/n$, $k = 0, \pm 1, \dots, \pm n$, i.e.,

$$\tilde{f}(t) = \frac{\lambda e^{\sigma t}}{2n} \sum_{-n}^n e^{\lambda \alpha_k t} (-i \cot \theta_k + i \theta_k \csc^2 \theta_k + 1) e^{i \lambda t \theta_k} \bar{f}(\lambda s_k + \sigma). \quad (6.7)$$

Writing

$$\bar{f}(\lambda s_k + \sigma) = G_k + iH_k, \quad (6.8)$$

where G_k and H_k are real, and noting that α_k is unchanged if k is replaced by $-k$ and $\tilde{f}(t)$ must be real, it follows that (6.7) takes the real form

$$\tilde{f}(t) = \frac{\lambda e^{\sigma t}}{n} \sum_{k=0}^n ' e^{\lambda \alpha_k t} \{ (G_k - \beta_k H_k) \cos \lambda t \theta_k - (H_k + \beta_k G_k) \sin \lambda t \theta_k \}, \quad (6.9)$$

where the prime indicates that the term $k = 0$ in the summation has to be multiplied by the factor $\frac{1}{2}$ and

$$\beta_k = \theta_k + \alpha_k(\alpha_k - 1)/\theta_k. \quad (6.10)$$

Note that because of the requirement (ii) the value of f will be zero when $k = n$ and thus the summation in (6.9) is effectively from 0 to $n - 1$. This is the basis of the method and, by carrying out an error analysis on the lines of Green, Talbot was able to choose the parameters n, λ and σ and get very accurate results for $f(t)$ for a wide variety of $\bar{f}(s)$.

6.2 A more general formulation

The subsequent paper by Talbot, although it was still modelled closely on that of Green, outlined a more general approach apart from the rotation of an auxiliary complex plane through a right angle for greater convenience. Let $z = x + iy$ be a complex variable and denote by M the interval from $z = -2\pi i$ to $z = 2\pi i$. Further, let $s = S(z)$ be a real uniform analytic function of z which

- (a) has simple poles at $\pm 2\pi i$, and residues there with imaginary parts respectively positive and negative;
- (b) has no singularities in the strip $|y| < 2\pi$;
- (c) maps M 1 - 1 onto a contour \mathfrak{B}' traversed upwards in the s -plane, which encloses all singularities of $f(\lambda s + \sigma)$ for some λ and σ ;
- (d) maps the half-strip $H : x > 0, |y| < 2\pi$ into the exterior of \mathfrak{B}' .

Then (6.3) holds and can be written as

$$f(t) = \frac{1}{2\pi i} \int_M Q(z) dz = \frac{1}{2\pi} \int_{-2\pi}^{2\pi} Q(iy) dy, \quad (6.11)$$

where

$$Q(z) = \lambda e^{(\lambda S + \sigma)t} \bar{f}(\lambda S + \sigma) S'(z). \quad (6.12)$$

As $z \rightarrow \pm 2\pi i$ on M we have $\Re s \rightarrow -\infty$ by virtue of (a) and (c) and, invoking (ii), we have $Q(\pm 2\pi i) = 0$. We note further that condition (c) depends on $\bar{f}(s)$ as well as S and cannot be satisfied if $\bar{f}(s)$ has an infinite number of singularities with imaginary parts extending to infinity. We can proceed as in the previous section to get a trapezoidal approximation $\tilde{f}(t)$ to $f(t)$ from (6.11) which is

$$\tilde{f}(t) = \frac{2}{n} \sum_{k=0}^{n-1} {}', \Re Q(z_k), \quad z_k = 2k\pi i/n \quad (6.13)$$

which is the general inversion formula considered by Talbot.

One particularly attractive feature of Talbot's method is the fact that we can estimate the error in $\tilde{f}(t)$. For, consider M_1 and M_2 to be any other two paths in the half-strip H the former to the right of M and the latter to the left of M but close enough to M to exclude any singularities of $f(\lambda S(z) + \sigma)$ and hence of $Q(z)$. Then

$$\tilde{f}(t) = \frac{1}{2\pi i} \int_{M_1 - M_2} \frac{Q(z) dz}{1 - e^{-nz}} \quad (6.14)$$

since the residue at $z = z_k = 2k\pi i/n$, $k = 0, \pm 1, \dots, \pm(n-1)$ is

$$\lim_{z \rightarrow z_k} \frac{(z - z_k)Q(z)}{1 - e^{-nz}} = \frac{Q(z_k)}{n}.$$

Note that the integrand is regular at $\pm 2\pi i$.

Now, by the assumptions (c) and (d), M in (6.11) may be replaced by the equivalent path M_1 . If we then combine (6.11) and (6.14) we obtain

$$\tilde{E}(t) = E_1(t) + E_2(t) \quad (6.15)$$

where $\tilde{E}(t)$ is the theoretical error (which depends on S, λ, σ and n as well as t) given by

$$\tilde{E}(t) = \tilde{f}(t) - f(t), \quad (6.16)$$

$$E_1(t) = \frac{1}{2\pi i} \int_{M_1} \frac{Qdz}{e^{nz} - 1} \quad (6.17)$$

and

$$E_2(t) = \frac{1}{2\pi i} \int_{M_2} \frac{Qdz}{1 - e^{-nz}} \quad (6.18)$$

Since $\Re z > 0$ on M_1 it is reasonable to assume that $E_1 \rightarrow 0$ as $n \rightarrow \infty$. In fact, Talbot establishes in his paper that if n is large enough we have

$$|E_1(t)| = O(n^2 \exp(h\tau - b\sqrt{\tau n} + \sigma t)), \quad (6.19)$$

where h and b are constants and $\tau = \lambda t$, in a region U which consists of the conjugate triangles ABC and ABD where C is the point $z = 2\pi i$ and D is the point $z = -2\pi i$. If M_1 is taken to lie inside U (see figure 6.1) then $E_1(t) \rightarrow 0$ as $n \rightarrow \infty$. Similarly, by taking M_2 to lie in a region U which is to the right of all singularities of $\tilde{f}(\lambda S + \sigma)$ we can establish that $E_2(t) \rightarrow 0$ as $n \rightarrow \infty$. This may have the effect of increasing h and decreasing b in (6.19) and hence increasing E_2 if $\tilde{f}(\lambda s + \sigma)$ has singularities near to \mathfrak{B}' .

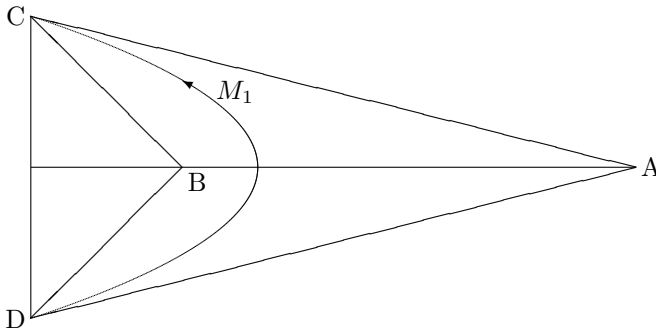
Thus for fixed t, λ and σ ,

$$\tilde{E} \rightarrow 0 \quad \text{as } n \rightarrow \infty. \quad (6.20)$$

Clearly from (6.19) the rate of convergence and the magnitude of \tilde{E} will depend greatly on τ .

In addition to the theoretical error we also have to ascertain the extent of the computational round-off error. From (6.12) and (6.13) it is clear that because of the exponential factor in Q , the first term in (6.13), namely

$$T_0 = \frac{\lambda}{n} \exp((\lambda S(0) + \sigma)t) \tilde{f}(\lambda S(0) + \sigma) S'(0), \quad (6.21)$$

Figure 6.1: The region U

is normally the largest or near-largest. Talbot found that because of heavy cancellation in the summation that $|\tilde{f}| \ll |T_0|$. Thus if the computer evaluates T_0 and its neighbouring values correct to c significant figures the rounding error E_r in \tilde{f} is roughly given by

$$E_r = O(10^{-c}T_0), \quad (6.22)$$

all other round-off errors in the evaluation being negligible by comparison. Thus the actual error in \tilde{f} is

$$E = E_1 + E_2 + E_r, \quad (6.23)$$

and from (6.20) it follows that $E = O(10^{-c}T_0)$ for sufficiently large n . This gives an asymptotic order of magnitude for the error which cannot be improved upon given a particular choice of λ and σ and contour \mathfrak{B}' .

6.3 Choice of Parameters

We shall include under this heading the choice of mapping function $S(z)$ and the parameters n, λ and σ . All that is required for the mapping function is that it should satisfy the conditions (a) - (d). A possibility which Talbot did not explore fully is

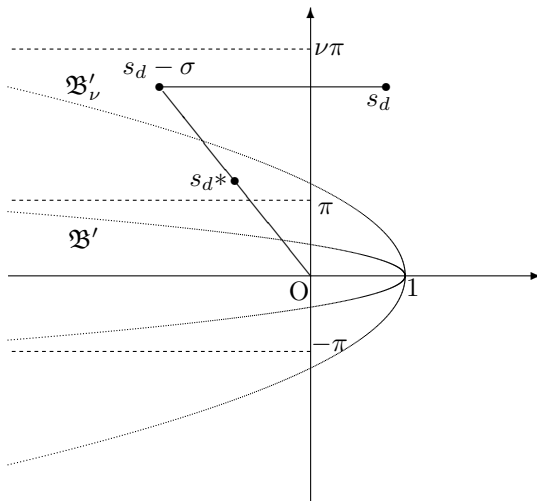
$$S(z) = az - \frac{b}{z^2 + 4\pi^2} + c.$$

He chose to consider the family of mappings

$$s = S_\nu(z) = \frac{z}{2} \left(\coth \frac{z}{2} + \nu \right) = \frac{z}{1 - e^{-z}} + az, \quad (6.24)$$

where ν is an arbitrary positive parameter and $a = (\nu - 1)/2$.

The singularities of $S_\nu(z)$ are simple poles at $\pm(2, 4, 6, \dots)\pi i$, and those at $\pm 2\pi i$

Figure 6.2: The contours \mathfrak{B}' and \mathfrak{B}'_ν

have residues $\pm 2\pi i$. $S_\nu(z)$ maps the interval $M(-2\pi i, 2\pi i)$ onto a contour

$$\mathfrak{B}'_\nu : s = s_\nu(\theta) = \alpha + \nu i\theta, \quad -\pi < \theta < \pi, \quad (6.25)$$

where $z = 2i\theta$ on M , and

$$\alpha = \alpha(\theta) = \theta \cot \theta. \quad (6.26)$$

The case $\nu = 1$ ($a = 0$) corresponds to the curve \mathfrak{B}' of the previous section. When $\nu \neq 1$, \mathfrak{B}'_ν consists of \mathfrak{B}' expanded vertically by a factor ν (see Figure 6.2) and there are advantages in taking $\nu > 1$.

With the choice of $S_\nu(z)$ given by (6.24) equation (6.9) now takes the form

$$\tilde{f}(t) = \frac{\lambda e^{\sigma t}}{n} \sum_{k=0}^{n-1} ' e^{\alpha \tau} \{ (\nu G_k - \beta H_k) \cos \nu \theta_k \tau - (\nu H_k + \beta G_k) \sin \nu \theta_k \tau \}, \quad (6.27)$$

where G, H and β are defined in (6.8) and (6.10).

We now give a strategy for the choice of the “geometrical” parameters λ, σ, ν for given $\bar{f}(s), t$, and computer precision c (as defined by (6.22)) and the selection of n for prescribed accuracy. First, we note that

1. If $\bar{f}(s)$ has no singularities in the half-plane $\Re s > 0$, then the inverse $f(t)$ may be expected to be $O(1)$, since \mathfrak{B} may be taken as the imaginary axis, possibly indented, and condition (ii) implies that $|\bar{f}(s)| \rightarrow 0$ at both ends of \mathfrak{B} .

2. If $\bar{f}(s)$ has singularities in the half-plane $\Re s > 0$ and \hat{p} is their maximum real part, then $f(t) = e^{\hat{p}t} \mathcal{L}^{-1} \bar{f}(s + \hat{p})$, where $\bar{f}(s + \hat{p})$ is of the type referred to in statement 1 (above), so that $f(t)$ is of order $O(e^{\hat{p}t})$, $\hat{p} > 0$.

Now suppose that the singularities of $\bar{f}(s)$ are at $s_j = p_j + iq_j$ and, as above, let

$$\hat{p} = \max_j p_j. \quad (6.28)$$

Next, write

$$\sigma_0 = \max(0, \hat{p}), \quad (6.29)$$

and apply an *initial shift* σ_0 to $\bar{f}(s)$. Then the the resulting function

$$\bar{f}_0(s) = \bar{f}(s + \sigma_0), \quad (6.30)$$

is always of type 1. Talbot's strategy was to produce an absolute error in $\tilde{f}_0(t)$ of order 10^{-D} , where D is specified, which produces a like error in $\tilde{f}(t)$ if $\bar{f}(s)$ is of type 1 and D correct significant digits if $\bar{f}(s)$ is of type 2. By the application of the shift σ_0 the singularities of $\bar{f}_0(s)$ will be at

$$s'_j = s_j - \sigma_0 = p'_j + iq_j, \quad p'_j = p_j - \sigma_0 \leq 0. \quad (6.31)$$

The strategy as applied to $\bar{f}_0(s)$ will involve a further shift, call it σ' (which may be zero) making a total shift σ such that

$$\sigma = \sigma' + \sigma_0. \quad (6.32)$$

After applying the initial shift σ_0 the next step is to find the "dominant" singularity of $\bar{f}(s)$, assuming that there are some complex singularities. If s_j is one of these, with $q_j > 0$, then the radius from the origin to the corresponding s'_j meets \mathfrak{B}' at a point where the ordinate is $\theta_j = \arg s'_j$. Thus s'_j is situated (q_j/θ_j) times as far out as that point, and we define the dominant singularity s_d to be the one for which this ratio is greatest, i.e. $s_d = p_d + iq_d$ satisfies

$$\frac{q_d}{\theta_d} = \max_{q_j > 0} \frac{q_j}{\theta_j}, \quad (6.33)$$

where

$$\theta_j = \arg s'_j. \quad (6.34)$$

If, however, all the singularities are real then they do not affect the choice of λ, σ, ν and there is no need to find a dominant singularity for this purpose although it is convenient to write $q_d = 0$ and $\theta_d = \pi$ in this case.

It follows from (6.22), because of the factor T_0 , that the round-off error is linked to

$$\omega = (\lambda + \sigma')t, \quad (6.35)$$

where σ has been replaced by σ' , as explained. Talbot asserts that experiments have shown that a correct choice of ω is vital for an efficient strategy and also that the optimum strategy depends on the value of v , where

$$v = q_d t. \quad (6.36)$$

There are two distinct cases to consider.

$$\text{Case 1.} \qquad v \leq \omega \theta_d / 1.8. \qquad (6.37)$$

In this situation we use only the initial shift σ_0 and a scaling factor λ but do not expand \mathfrak{B}' ; we take

$$\left. \begin{aligned} \lambda &= \omega/t & (\tau = \omega), \\ \sigma &= \sigma_0 & (\sigma' = 0), \\ \nu &= 1 & (a = 0), \end{aligned} \right\} \qquad (6.38)$$

and note that with this choice (6.35) is satisfied. Case 1 always occurs when the singularities of $\bar{f}(s)$ are all real.

$$\text{Case 2.} \qquad v > \omega \theta_d / 1.8. \qquad (6.39)$$

In this case we use the expanded contour \mathfrak{B}'_ν , as shown in Fig. 6.2. With ϕ as defined in the figure,

$$p_d - \sigma = \frac{q_d}{\nu} \cot \phi. \qquad (6.40)$$

If λ_ν is the value of λ which would bring $s_d - \sigma$ just onto \mathfrak{B}'_ν then

$$\lambda_\nu = q_d / \nu \phi. \qquad (6.41)$$

If we define κ to be the ratio λ / λ_ν , which quantifies how far s_d^* is inside \mathfrak{B}'_ν then

$$\kappa = \nu \lambda \phi / q_d. \qquad (6.42)$$

Finally, if we regard ω, ϕ, κ as three new parameters we can solve (6.35), (6.40) and (6.42) for λ, σ, ν and obtain

$$\lambda = \kappa q_d / \nu \phi, \quad \sigma = p_d - \frac{q_d}{\nu} \cot \phi, \quad \nu = q_d \left(\frac{\kappa}{\phi} - \cot \phi \right) / \left(\frac{\omega}{t} + \sigma_0 - p_d \right).$$

Talbot remarks that better results are obtained if we replace p_d by \hat{p} (thus ensuring $\sigma' > 0$) in which case our formulae in Case 2 become

$$\left. \begin{aligned} \lambda &= \kappa \mu / \phi, \\ \sigma &= \hat{p} - \mu \cot \phi, \\ \nu &= q_d / \mu, \end{aligned} \right\} \qquad (6.43)$$

where

$$\mu = \left(\frac{\omega}{t} + \sigma_0 - \hat{p} \right) / \left(\frac{\kappa}{\phi} - \cot \phi \right). \qquad (6.44)$$

Satisfactory values of κ, ϕ and ω were found to be

$$\left. \begin{aligned} \kappa &= 1.6 + 12/(v + 25), \\ \phi &= 1.05 + 1050/\max(553, 800 - v), \\ \omega &= \min(0.4(c + 1) + v/2, 2(c + 1)/3). \end{aligned} \right\} \quad (6.45)$$

Finally, Talbot presents empirical criteria for choosing n to achieve D significant figure accuracy (if $\hat{p} > 0$) or error in the D th decimal place (if $\hat{p} \leq 0$). We refer the reader to Talbot [227] for details. Suffice it to say that if all the singularities are real then only moderate values of n are needed to determine $\tilde{f}(t)$. In other cases the value of n will increase as t increases and it is probably easier to use an adaptive procedure for determining n .

6.4 Additional Practicalities

We list a number of points which were not discussed in previous sections.

1. Formula (6.27) requires the evaluation of $\cos \nu \theta_k \tau$ and $\sin \nu \theta_k \tau$ and this can give rise to an appreciable error as the argument can be of order 10^2 . We write (6.27) as

$$\tilde{f}(t) = \frac{\lambda e^{\sigma t}}{n} \Re \sum_0^{n-1} ' a_k e^{ki\psi}, \quad (6.46)$$

where

$$a_k = [e^{\alpha t}(\nu + i\beta)\bar{f}(\lambda s_\nu + \sigma)]_{\theta=\theta_k}, \quad \psi = \tau \nu \pi / n. \quad (6.47)$$

As the factors $e^{ki\psi}$ in (6.46) satisfy the same recurrence relation as the Chebyshev polynomials $T_k(\cos \psi)$, namely

$$e^{(k+1)i\psi} + e^{(k-1)i\psi} = 2 \cos \psi \cdot e^{ki\psi}, \quad (6.48)$$

it follows that the sum in (6.46) can be evaluated by an algorithm like that of Clenshaw for Chebyshev sums, viz.,

$$\left. \begin{aligned} b_{n+1} &= b_n = 0, \\ b_k &= a_k + ub_{k+1} - b_{k+2} \quad (u = 2 \cos \psi), \quad k = n-1, \dots, 1, \\ \sum ' &= \frac{1}{2}(a_0 + ub_1) - b_2 + ib_1 \sin \psi. \end{aligned} \right\} \quad (6.49)$$

In adopting the above algorithm we observe that the only trigonometrical evaluations required are those for $\cos \psi$ and $\sin \psi$ and thus, as well as increasing accuracy, this device saves time.

2. If $\bar{f}(s) = e^{-a/s}/\sqrt{s}$, for example, we have a function with an essential singularity at $s = 0$. Thus Case 1 applies with $\lambda = \omega/t$, $\tau = \omega$, $\sigma = 0$, $\nu = 1$ and $\omega = 0.4(c+1)$ so that λ will be small when t is large. Analysis indicates

that T_0 is not now the largest term and the largest term increases rapidly (almost exponentially) thus thwarting the general strategy regarding E_r . We can remedy the matter quite simply by setting a lower bound for λ , say, $\omega = 0.4(c+1) - 1 + at/30$. This would also be the case for any other transforms having $e^{-a/s}$ as a factor.

The problem does not arise if $a < 0$.

3. When there are complex singularities then the dominant singularity played an essential role in the Talbot strategy. For given t , the larger the imaginary part q_d the larger $v = q_d t$ becomes and this, in turn, means that n will have to be larger to obtain D digit accuracy. If however the position of s_d is known exactly and $q_d/\theta_d \gg$ like terms then n can be reduced significantly by applying the subdominant singularity $s_{d'}$ to determine the parameters λ, σ, ν and n and taking account of s_d by adding the residue term

$$e^{s_d t} \bar{f}(s_d) \quad (6.50)$$

to $\tilde{f}(t)$. We have to ensure, however, that with the chosen parameters, s_d^* lies outside \mathfrak{B}'_ν .

6.5 Subsequent development of Talbot's method

Talbot's method has been used by many authors to evaluate Laplace Transforms which have occurred in their work. Comparison of Talbot's method have also been made with other available techniques. There have also been modifications proposed which relate to the optimum choice of parameters which also includes choice of contour.

6.5.1 Piessens' method

Instead of Talbot's contour \mathfrak{B}'_ν Piessens takes a contour \mathcal{C} which consists of the straight lines $s = x - i\beta$, $-\infty < x \leq \alpha$; $s = \alpha + iy$, $-\beta \leq y \leq \beta$; $s = x + i\beta$, $-\infty < x < \alpha$ where α and β are chosen so that \mathcal{C} includes all singularities of the function $\bar{f}(s)$ as in Figure 6.3 . We now have

$$\begin{aligned} f(t) &= \frac{1}{2\pi i} \int_{\mathcal{C}} e^{st} \bar{f}(s) ds, \\ &= \int_{-\infty}^{\alpha} e^{t(x-i\beta)} \bar{f}(x-i\beta) dx + \int_{-\beta}^{\beta} e^{t(\alpha+iy)} \bar{f}(\alpha+iy) i dy \\ &\quad + \int_{\alpha}^{-\infty} e^{t(x+i\beta)} \bar{f}(x+i\beta) dx. \end{aligned} \quad (6.51)$$

The first and third integrals combine to give (apart from a constant factor)

$$I_1 = - \int_{-\infty}^{\alpha} e^{xt} [G(x+i\beta) \sin(\beta t) + H(x+i\beta) \cos(\beta t)] dx, \quad (6.52)$$

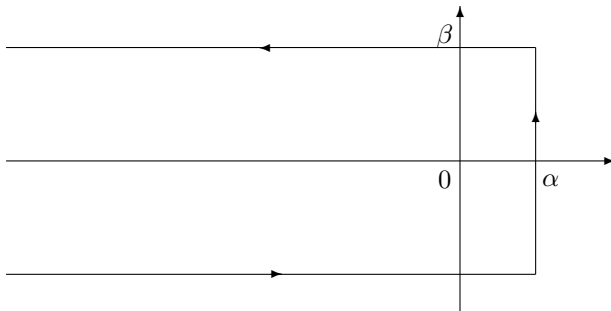


Figure 6.3: The Piessens contour

where

$$G(s) = \Re \bar{f}(s), \quad H(s) = \Im \bar{f}(s). \quad (6.53)$$

Likewise, the middle integral can be split into two parts I_2 and I_3 where, suppressing the factor $e^{\alpha t}$,

$$I_2 = \int_0^\beta G(\alpha + iy) \cos(ty) dy, \quad (6.54)$$

$$I_3 = - \int_0^\beta H(\alpha + iy) \sin(ty) dy. \quad (6.55)$$

Piessens makes the substitution $u = xt$ in the integrand I_1 to get

$$I_1 = -t^{-1} \int_{-\infty}^{\alpha t} e^u [G(u/t + i\beta) \sin(\beta t) + H(u/t + i\beta) \cos(\beta t)] du, \quad (6.56)$$

so that finally

$$f(t) = [e^{\alpha t}(I_2 + I_3) + I_1]/\pi. \quad (6.57)$$

For these integrals we cannot now use the trapezium rule, as Talbot had done, but have to resort to quadrature rules which are specifically designed for oscillatory integrals - Piessens uses the Fortran Routine DQAWO to evaluate I_1 and DQAGI to evaluate I_2 and I_3 (see Piessens et al [185]). He also mentions that it is better to keep the values of α and β small, especially for large t but at the same time one has to ensure that singularities are not too close to the contour \mathcal{C} . He suggests taking

$$\alpha = a + c_1/t, \quad \beta = b + c_2/t, \quad (6.58)$$

where c_1 and c_2 are constants such that $1 \leq c_1 = c_2 \leq 5$, a is the smallest value for which $\bar{f}(s)$ is analytic in $|\Re s| < a$ and b is the smallest value for which $\bar{f}(s)$

is analytic in $|\Im s| > b$. When $\bar{f}(s)$ has branch points Piessens stresses the need to choose the branch for which G and H are continuous along the contour as is the case when

$$\bar{f}(s) = (s^2 + 1)^{-\frac{1}{2}}, \quad f(t) = J_0(t). \quad (6.59)$$

6.5.2 The Modification of Murli and Rizzardi

Murli and Rizzardi [159], instead of using the algorithm (6.49) to sum the series

$$\sum_{k=1}^{n-1} a_k \sin k\psi \quad \text{and} \quad \sum_{k=0}^{n-1} a_k \cos k\psi,$$

employ the Goertzel-Reinsch algorithm which is based on the following result:-

Given $\psi (\neq r\pi)$, $r = 0, \pm 1, \pm 2, \dots$ and

$$U_j = \frac{1}{\sin \psi} \sum_{k=j}^{n-1} a_k \sin(k-j+1)\psi, \quad j = 0, 1, \dots, n-1$$

$$U_n = U_{n+1} = 0$$

then

$$U_j = a_j + 2(\cos \psi)U_{j+1} - U_{j+2}, \quad j = n-1, n-2, \dots, 0$$

and

$$S = \sum_{k=1}^{n-1} a_k \sin k\psi = U_1 \sin \psi$$

$$C = \sum_{k=0}^{n-1} a_k \cos k\psi = a_0 + U_1 \cos \psi - U_2.$$

The GR algorithm is:-

Define

$$\Delta_\omega U_j = U_{j+1} - \omega * U_j,$$

where

$$\omega = \operatorname{sgn}(\cos \psi),$$

and

$$\lambda = \begin{cases} -4 \sin^2(\psi/2) & \text{if } \omega > 0 \\ 4 \cos^2(\psi/2) & \text{if } \omega \leq 0 \end{cases}$$

Set

$$U_{n+1} = \Delta_\omega U_n = 0.$$

do $j = (n - 1), 0, -1$

$$\begin{aligned} U_{j+1} &= \Delta_\omega U_{j+1} + \omega U_{j+2} \\ \Delta_\omega U_j &= \lambda U_{j+1} + \omega \Delta_\omega U_{j+1} + a_j \end{aligned}$$

enddo

yielding

$$\begin{aligned} S &= U_1 \sin \psi \\ C &= \Delta_\omega U_0 - (\lambda/2)U_1 \end{aligned}$$

They also have some other modifications which are included in their published routine Algorithm 682 in the ACM Transactions (TOMS). A condensed version of their routine is provided at the URL www.cf.ac.uk/maths/cohen/programs/inverselaplace transform/.

6.5.3 Modifications of Evans et al

Since it is possible to obtain good results for the evaluation of oscillatory integrals over a finite range Evans [80] had the idea of choosing a contour which is defined in terms of J piece-wise contours so that now

$$\mathfrak{B}' = \bigcup_1^J \mathfrak{B}_j, \quad (6.60)$$

where

$$\mathfrak{B}_j : s = \alpha_j(\tau) + i\beta_j(\tau), \quad (6.61)$$

and $\alpha_j(\tau)$ may be any continuous function but $\beta_j(\tau)$ is restricted to a linear form $\beta_j(\tau) = m_j\tau + c_j$. Thus, on a sub-contour \mathfrak{B}_j , we will need to evaluate

$$\frac{1}{2\pi i} \int \bar{f}(\alpha + i\beta) e^{t(\alpha + i\beta)} (d\alpha + id\beta).$$

Writing $\bar{f}(s) = G(s) + iH(s)$, as before, this reduces to

$$\frac{1}{2\pi} \left\{ \int e^{t\alpha} [G \sin t\beta + H \cos t\beta] d\alpha + \int e^{t\alpha} [G \cos t\beta - H \sin t\beta] d\beta \right\}.$$

Now, substitution of the linear form for β gives

$$\begin{aligned} & \frac{1}{2\pi} \int_{\mathfrak{B}_j} e^{t\alpha} [(G\beta' + H\alpha') \cos tc + (G\alpha' - H\beta') \sin tc] \cos mt\tau d\tau \\ & + \frac{1}{2\pi} \int_{\mathfrak{B}_j} e^{t\alpha} [(G\alpha' - H\beta') \cos tc - (G\beta' + H\alpha') \sin tc] \sin mt\tau d\tau, \end{aligned} \quad (6.62)$$

and thus the integral over the sub-contour involves two standard oscillatory integrals. Evans points out an advantage of taking the contour to be piece-wise linear as the same G and H values can be used in the two integrals in (6.62) and, if the contour is symmetrical about the x -axis the first and last sections of the contour will run parallel to the real axis and will not be oscillatory. Hence for these sections a general purpose quadrature rule, such as that of Clenshaw-Curtis [40] will be viable. The term $e^{t\alpha} \rightarrow 0$ as $\alpha \rightarrow -\infty$ and this ensures that the integration need only be performed over a limited section of these parallel contours. In fact if we curtail the integration when $\alpha = -32/t$ we are guaranteed 14 figure accuracy. Evans proposes four contours which can be used for comparison purposes. The first consists of the sub-contours

$$\begin{aligned} \mathfrak{B}_1 : s &= x - ib_1, \quad -\infty < x < a_1, \\ \mathfrak{B}_2 : s &= x + ib_1(x - a_0)/(a_0 - a_1), \quad a_1 \leq x \leq a_0, \\ \mathfrak{B}_3 : s &= x + ib_1(x - a_0)/(a_1 - a_0), \quad a_0 \geq x \geq a_1, \\ \mathfrak{B}_4 : s &= x + ib_1, \quad a_1 > x > -\infty. \end{aligned}$$

The second contour is the contour \mathfrak{B}'_ν used by Talbot, the third is given by

$$\alpha = c - \frac{b}{4(\pi^2 - \tau^2)}, \quad \beta = 2a\tau$$

(which was suggested as a possibility by Talbot but not used) and, finally,

$$\alpha = c - a\tau^n, \quad \beta = b\tau,$$

where the constants are chosen to correspond with a_0 , a_1 and b_1 for the piece-wise straight line contour. Thought has to be given to the choice of these quantities as one needs the contour to be sensibly positioned in relation to the dominant singularity.

Evans points out that there is a significant advantage in choosing a piece-wise linear contour as it makes it easy to automate the process. This can be done in three steps:-

- (i) Order the poles into ascending argument (after first arranging for all the poles to lie just above or on the real axis).
- (ii) Compute the gradients of the lines joining successive points in the ordered list from step (i).

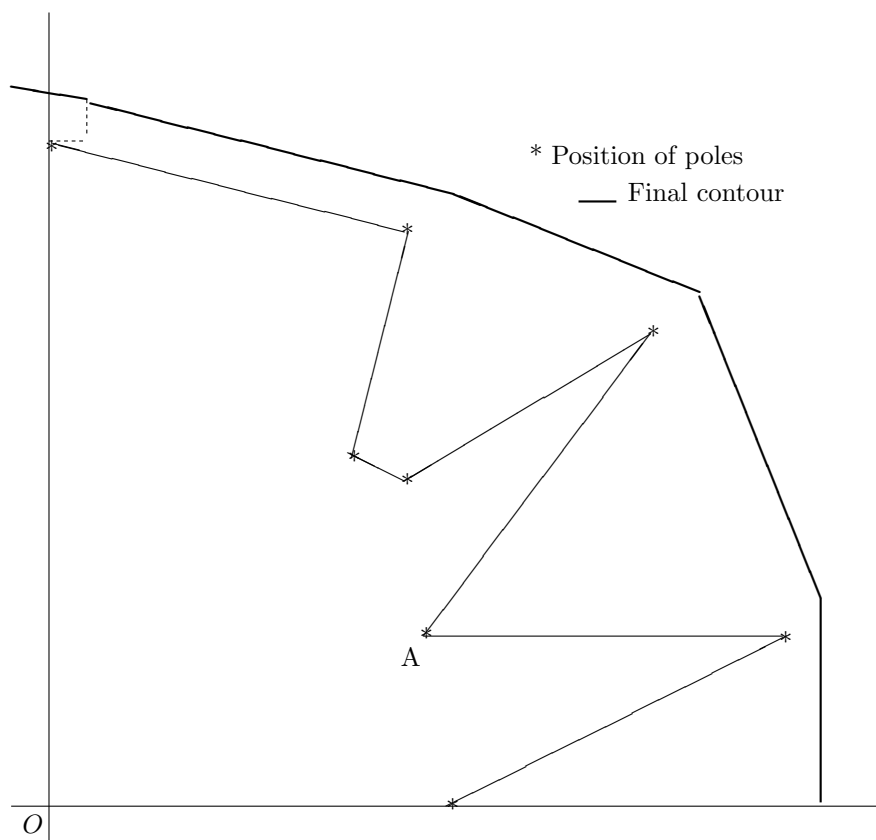


Figure 6.4: The Evans contour

- (iii) Scan through the list of gradients starting from the positive real axis. If a gradient is greater than its predecessor then move on to the next gradient, otherwise, reject the pole at the lower end of the line as, for example, A in Fig. 6.4. The process is repeated until there are no rejections.

We have effectively found an “envelope” for the poles and we complete the process by adding a small distance ε to the real and imaginary parts of the accepted points so that the final contour consists of line segments which are just to the right of the “envelope” and thus the contour will contain all the poles. The contour is started by a leg running parallel to the real axis from $-\infty$ to the pole with least imaginary part and ends with a leg from the pole with maximum imaginary part to $-\infty$ which is also parallel to the axis. If the poles are all real then a contour similar to that of the Piessens contour \mathcal{C} is used.

In a subsequent development Evans and Chung [82] employ ‘optimal contours’ \mathcal{C} to deform the Bromwich contour. One choice of \mathcal{C} , which may not be optimal, possesses the following properties:-

- (i) \mathcal{C} consists of two branches \mathcal{C}_1 and \mathcal{C}_2 where \mathcal{C}_1 lies in the upper half-plane and \mathcal{C}_2 in the lower half-plane and the two branches meet at only one point on the real axis ($\Re s = a$). The contour \mathcal{C} is to be traversed in an anticlockwise manner.
- (ii) Both \mathcal{C}_1 and \mathcal{C}_2 extend to infinity in the half-plane $\Re s \leq a$.
- (iii) There may be poles of $\bar{f}(s)$ to the right of \mathcal{C} but all essential singularities and branch points of $\bar{f}(s)$ lie to the left of \mathcal{C} with no poles on \mathcal{C} .

Evans and Chung note that if $\bar{f}(s)$ is real when s is real and \mathcal{C} satisfies the conditions (i) and (iii) and is symmetrical about the real axis then

$$\frac{1}{2\pi i} \int_{\mathcal{C}} e^{ts} \bar{f}(s) ds = \frac{1}{\pi} \Im \int_{\mathcal{C}_1} e^{ts} \bar{f}(s) ds,$$

where \mathcal{C}_1 is the upper branch of \mathcal{C} . They then set about finding an optimal contour for

$$\int_{\mathcal{C}} e^{ts} \bar{f}(s) ds$$

by assuming that the oscillation in the integrand comes mainly from the factor e^{ts} where t is fixed and positive. With $s = \alpha + i\beta$ we have

$$e^{ts} = e^{t(\alpha+i\beta)} = e^{t\alpha} e^{it\beta},$$

and by setting

$$t\beta = \text{constant},$$

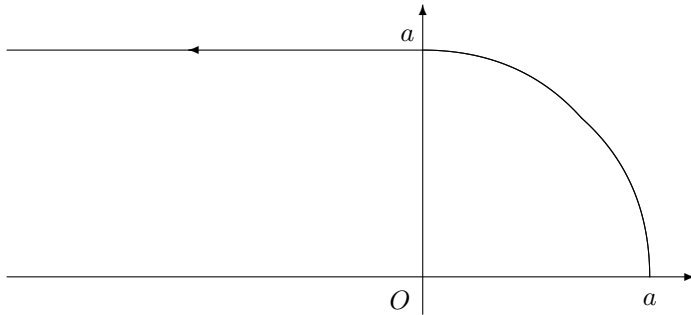
we can eliminate the oscillation. The steepest curves are thus the horizontal lines $\beta = \text{constant}$. As the contour \mathcal{C}_1 must start on the axis the horizontal line cannot be used on its own without the addition of a curve of finite length running from the axis and joining it at some point. The authors took the quarter circle $s = a$ joining on to the line $\Im s = a$ to constitute the optimal contour (see Figure 6.5). Thus in polar coordinates we have

$$\mathcal{C}_1 : r = \begin{cases} a, & a \leq \theta \leq \pi/2; \\ a/\sin \theta, & \pi/2 < \theta < \pi. \end{cases} \quad (6.63)$$

An appropriate choice for a is

$$a = \pi/2t \quad (6.64)$$

since, as we move on the circular arc the oscillatory factor $e^{it\beta}$ changes only through a quarter of a cycle and is effectively non-oscillatory over this arc.

Figure 6.5: The (optimal) contour \mathcal{C}_1

To avoid the contour passing through some singularities Evans and Chung introduce a real shift parameter σ defined by

$$\sigma = \max \Re s_k + \varepsilon$$

where the maximum is taken over all singularities s_k of $\bar{f}(s)$ and $\varepsilon = 1/t$ if there is a singularity lying exactly on \mathcal{C} and $\varepsilon = 0$ otherwise. We can now employ the result (2.22) of Chapter 2 to obtain

$$f(t) = \frac{e^{t\sigma}}{\pi} \oint_{\mathcal{C}} \bar{f}(s + \sigma) e^{ts} ds + \sum_k R_k \quad (6.65)$$

where R_k denotes the residue at the pole s_k of the function $e^{ts} \bar{f}(s)$.

6.5.4 The Parallel Talbot Algorithm

The previous implementations of Talbot's method have been designed for sequential computers. de Rosa et al [66] state that these have been efficient for moderate t as few (Laplace transform) function evaluations are needed. For large t thousands of function evaluations may be required to ensure high accuracy of the result. They produce a parallel version of Talbot's method to achieve a faster inversion process.

A core feature of their approach is the incorporation of the Goertzel-Reinsch algorithm used by Murli and Rizzardi [159]. de Rosa et al assume that p parallel computers are available, where for simplicity n is a multiple of p , and they divide S and \mathcal{C} into p independent subsequences. These are computed independently by each processor and a single global sum is all that is needed to accumulate the p local partial results. Thus if

$$n_p = n/p$$

and we set

$$\Phi_{r_j}^{r_{j+1}} = \sum_{k=r_j}^{r_{j+1}-1} a_k \sin k\psi \quad (6.66)$$

$$\Gamma_{r_j}^{r_{j+1}} = \sum_{k=r_j}^{r_{j+1}-1} a_k \cos k\psi \quad (6.67)$$

$$(6.68)$$

where $r_j = jn_p$ for $j = 0, 1, \dots, p-1$
then

$$S = \sum_{j=0}^{p-1} \Phi_{r_j}^{r_{j+1}} \quad (6.69)$$

$$C = \sum_{j=0}^{p-1} \Gamma_{r_j}^{r_{j+1}} \quad (6.70)$$

The task of processor ‘ j ’ is then to compute the sums in (6.66) and (6.67). de Rosa et al note that if the sums to be computed are

$$\begin{aligned} \Phi_j^n &= \sum_{k=j}^{n-1} a_k \sin k\psi \\ \Gamma_j^n &= \sum_{k=j}^{n-1} a_k \cos k\psi, \quad j = 0, 1, \dots, n-1 \end{aligned}$$

and we set

$$\begin{aligned} A_j^n &= \sum_{k=j}^{n-1} a_k \sin(k-j)\psi \\ B_j^n &= \sum_{k=j}^{n-1} a_k \cos(k-j)\psi \end{aligned}$$

then

$$\begin{aligned} \Phi_j^n &= A_j^n \cos j\psi + B_j^n \sin j\psi \\ \Gamma_j^n &= B_j^n \cos j\psi - A_j^n \sin j\psi, \quad j = 0, 1, \dots, n-1 \end{aligned}$$

6.6 Multi-precision Computation

We have already remarked that inversion of the Laplace transform is an ill-conditioned problem. This certainly manifests itself in numerical methods

with loss of numerical digits brought about by cancellation. As with other ill-conditioned problems, such as the solution of the simultaneous linear equations $H\mathbf{x} = \mathbf{b}$ where H is the Hilbert matrix with elements $h_{ij} = 1/(i + j - 1)$, accurate answers are obtainable for \mathbf{x} if we use extended precision arithmetic.

Abate and Valkó have adopted this brute force computational approach to obtain what they term the fixed-Talbot method. Clearly, as they do not have to concern themselves with having to achieve the maximum computational efficiency by, for example, using the Goertzel-Reinsch algorithm, they were able to use a shorter program. In fact, their *Mathematica* program consisted of just 10 lines. The basis of their formulation is, like Talbot, that the inverse transform is given by

$$f(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \bar{f}(s) ds. \quad (6.71)$$

The contour is deformed by means of the path

$$s(\theta) = r\theta(\cot \theta + i), \quad -\pi < \theta < \pi, \quad (6.72)$$

where r is a parameter. This path only involves one parameter whereas Talbot's consisted of two. Integration over the deformed path yields

$$f(t) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} e^{ts(\theta)} \bar{f}(s(\theta)) s'(\theta) d\theta. \quad (6.73)$$

Differentiating (6.72) we have $s'(\theta) = ir(1 + i\sigma(\theta))$, where

$$\sigma(\theta) = \theta + (\theta \cot \theta - 1) \cot \theta. \quad (6.74)$$

We find

$$f(t) = \frac{r}{\pi} \int_0^{\pi} \Re \left[e^{ts(\theta)} \bar{f}(s(\theta)) (1 + i\sigma(\theta)) \right] d\theta \quad (6.75)$$

Approximation of the integral in (6.75) by the trapezoidal rule with step size π/M and $\theta_k = k\pi/M$ yields

$$f(t, M) = \frac{r}{M} \left\{ \frac{1}{2} f(r) e^{rt} + \sum_{k=1}^{M-1} \Re [e^{ts(\theta_k)} \bar{f}(s(\theta_k)) (1 + i\sigma(\theta_k))] \right\}. \quad (6.76)$$

Based on numerical experiments Abate and Valkó chose r to be

$$r = 2M/(5t), \quad (6.77)$$

which results in the approximation $f(t, M)$ being dependent on only one free parameter, M . Finally to control round-off error they took the number of precision decimal digits to be M . An example of their *Mathematica* program is provided at the URL

www.cf.ac.uk/maths/cohen/programs/inverselaplacetransform/.

Valkó and Abate [238] have used the above algorithm as the inner loop of a program which inverts two-dimensional transforms — see Chapter 7.

Chapter 7

Methods based on the Post-Widder Inversion Formula

7.1 Introduction

In Chapter 2 we established the Post-Widder formula for the inversion of Laplace Transforms. One of the difficulties of using this particular approach is the need to differentiate $\bar{f}(s)$ a large number of times especially when it is a complicated function. However, with the general availability of Maple and Mathematica this isn't quite the headache it used to be. The other major problem with this approach to inversion lies with the slow convergence to the limit. To illustrate this point we have tabulated in Table 7.1

$$f_n(t) = \frac{(-1)^n}{n!} \left(\frac{n}{t}\right)^{n+1} \bar{f}^{(n)}\left(\frac{n}{t}\right), \quad (7.1)$$

where $\bar{f}(s) = 1/(s+1)$ for various n, t . Clearly when $n = 50$ the approximation for $f(1)$ is in error by about 1% while for $f(5)$ the error is about 15%. Because of the slow convergence of the sequence $f_n(t)$ it is natural to seek extrapolation methods to speed up convergence. As we point out in the section on Extrapolation in Chapter 11 there is no magic prescription which will enable one to sum all convergent sequences. Perhaps the most robust technique for achieving this is the $d^{(m)}$ -transformation as one can vary m , if need be, to obtain a more appropriate extrapolation technique. For the above example $m = 1$ was found to be sufficient to produce satisfactory results when using the Ford-Sidi $W^{(m)}$ algorithm with np=3 (a program can be downloaded from www.cf.ac.uk/maths/cohen/programs/inverselaplace/transform/). The ρ -algorithm was also very successful and produced results for $f(1)$ and $f(5)$ which were correct to 18 and 12 decimal places respectively using only 13 function values. With 19 function values we also obtained similar accuracy for $f(5)$.

n	$f_n(1)$	$f_n(5)$
1	0.250000000	0.027777...
2	0.296296...	0.023323...
5	0.334897...	0.015625000
10	0.350493...	0.011561...
20	0.358942...	0.009223...
50	0.364243...	0.007744...
Exact $f(t)$	0.367879...	0.006737...

Table 7.1: Crude approximations for $f(t)$ when $\bar{f}(s) = 1/(s+1)$.

n	$f_n(2)$
1	0.0894427191
2	0.0883883476
3	0.0920292315
4	0.1001758454
5	0.1096308396
6	0.1188238282
7	0.1271993514
8	0.1346391708
9	0.1411901193
10	0.1469511888
11	0.1520292063

Table 7.2: Crude approximations for $f(t)$ when $\bar{f}(s) = 1/\sqrt{s^2+1}$.

Moreover, we could compute $f(40)$ by this method correct to 24 decimal places. Of course, all calculations needed were performed using quadruple length arithmetic (approximately 32-digit decimal arithmetic) in order to achieve the required accuracy. For general $f(t)$ we might not have so many terms of the sequence available because of the difficulty in differentiating $\bar{f}(s)$.

Example 7.1 Given $\bar{f}(s) = 1/(s^2+1)^{1/2}$ estimate $f(t)$ for $t = 2$. We have

$$\bar{f}'(s) = -s/(s^2+1)^{3/2},$$

and thus

$$(s^2+1)\bar{f}'(s) + s\bar{f}(s) = 0.$$

This last equation can be differentiated n times by Leibnitz's theorem to get

$$(s^2+1)\bar{f}^{(n+1)}(s) + (2n+1)s\bar{f}^{(n)}(s) + n^2\bar{f}^{(n-1)}(s) = 0.$$

If we now substitute $s = n/t$ we can, for each n , compute the terms $f_n(t)$ given by (7.1). These are given in Table 7.2 .

It is difficult to decide whether this data is converging but if, as before, we apply the ρ -algorithm we obtain the estimate 0.22389079 for $f(2)$. The exact answer is $J_0(2) = 0.2238907791 \dots$.

On a parallel computer it would of course be possible to obtain estimates for several values of t simultaneously the only limitation being numerical instability caused by loss of significant digits. A different approach to applying the Post-Widder formula has been given by Jagerman [116], [117].

7.2 Methods akin to Post-Widder

Davies and Martin [60] give an account of the methods they tested in their survey and comparison of methods for Laplace Transform inversion. Their conclusions were that the Post-Widder method seldom gave high accuracy — as we confirmed with the examples in the previous section — but, apart from the ϵ -algorithm which they mention, there were very few extrapolation techniques which were well-known at that time. The power of extrapolation techniques is demonstrated convincingly by the examples we give in this and other chapters. Davies and Martin in their listing of *methods which compute a sample* give the formula

$$I_n(t) = \int_0^\infty \delta_n(t, u) f(u) du, \quad (7.2)$$

where the functions $\delta_n(t, u)$ form a delta convergent sequence, and thus $I_n(t)$ tends to $f(t)$ with increasing n . The Post-Widder formula may be thought of as being obtained from the function

$$\delta_n(t, u) = (nu/t)^n \exp(-nu/t)/(n-1)!.$$

Using a similar approach ter Haar [228] proposed the formula

$$f(t) \approx t^{-1} \bar{f}(t^{-1}), \quad (7.3)$$

and another variant due to Schapery [205] is

$$f(t) \approx (2t)^{-1} \bar{f}((2t)^{-1}). \quad (7.4)$$

As these last two formulae are essentially just the first terms in a slowly convergent sequence we cannot really expect them to provide accurate results. Gaver [93] has suggested the use of the functions

$$\delta_n(t, u) = \frac{(2n)!}{n!(n-1)!} a(1 - e^{-au})^n e^{-nau}, \quad (7.5)$$

where $a = \ln 2/t$, which yields a similar result to (7.1) but involves the n th finite difference $\Delta^n f(na)$, namely,

$$f(t) = \lim_{n \rightarrow \infty} I_n(t) = \lim_{n \rightarrow \infty} \frac{(2n)!}{n!(n-1)!} a \Delta^n \bar{f}(na). \quad (7.6)$$

n	I_n
1	0.237827565897
2	0.288305006172
3	0.310487554891
4	0.322983551879
5	0.331006106802
6	0.336594259156
7	0.340710666619
8	0.343869331482
9	0.346369783782
10	0.348398408180
11	0.350077271302

Table 7.3: Successive Gaver iterates for $f(t)$ when $\bar{f}(s) = 1/(s+1)$.

As with the Post-Widder formula the convergence of $I_n(t)$ to $f(t)$ is slow. However, we can try and speed things up by application of extrapolation techniques. Gaver has shown that $(I_n(t) - f(t))$ can be expanded as an asymptotic expansion in powers of $1/n$ which gives justification for using this approach. Stehfest [224], [225] gives the algorithm

$$f(t) \approx a \sum_{n=1}^N K_n \bar{f}(na), \quad a = \ln 2/t, \quad (7.7)$$

where N is even and

$$K_n = (-1)^{n+N/2} \sum_{k=\lceil (n+1)/2 \rceil}^{\min(n, N/2)} \frac{k^{N/2} (2k)!}{(N/2 - k)! k! (k-1)! (n-k)! (2k-n)!},$$

and this formula has been used by Barbuto [12] using a Turbo Pascal 5.0 program to determine the numerical value of the inverse Laplace transform of a Laplace-field function. Davies and Martin [60] report that this method gives good accuracy on a wide range of functions. We have used the Gaver formula (7.6) to estimate $f(t)$ given that $\bar{f}(s) = 1/(s+1)$ and we obtained the approximations (Table 7.3) for $I_n(t)$ when $t = 1$. We remark that the term $I_n(t)$ in (7.6) can be obtained by means of the recursive algorithm

$$\left. \begin{aligned} G_0^{(n)} &= na \bar{f}(na), \quad n \geq 1 \\ G_k^{(n)} &= \left(1 + \frac{n}{k}\right) G_{k-1}^{(n)} - \frac{n}{k} G_{k-1}^{(n+1)}, \quad k \geq 1, n \geq k \\ I_n(t) &= G_n^{(n)} \end{aligned} \right\} \quad (7.8)$$

— see Gaver [93] and also Valkó and Abate [237]. As before, we have used quadruple length arithmetic to compute the data in the above table (which gives the rounded values correct to 12 decimal places). Again, it is difficult to decide

what the sequence is converging to (if it is converging at all). Application of the ρ -algorithm to the data in the above table yielded the value $0.3678794411708 \dots$ which is the correct value of e^{-1} to 11 significant figures. When t is increased we have to increase n in order to achieve the same sort of accuracy but this leads to loss of digits in I_n due to cancellation so that we cannot get even 6 significant digit accuracy for $t > 15$. Of course, we might be less successful with the extrapolation if we are given some other function $\bar{f}(s)$ but could try some other extrapolation technique such as the Ford- Sidi $W^{(m)}$ algorithm. Nevertheless, where it is difficult to compute the derivatives of $\bar{f}(s)$, and this is frequently the case, the Gaver method is an attractive alternative to Post-Widder.

Another approach which does not seem to have been implemented is to use the inversion formula of Boas and Widder [21]

$$f(t) = \lim_{k \rightarrow \infty} f_k(t),$$

where

$$f_k(t) = \frac{t^{k-1}}{k!(k-2)!} \int_0^\infty \frac{\partial^k}{\partial s^k} [s^{2k-1} e^{-ts}] \bar{f}(s) ds. \quad (7.9)$$

If parallel computation facilities are available $f_k(t)$ can be computed simultaneously for each $k = 1, 2, \dots$, the integral being determined using methods given in Chapter 11, and then we can extrapolate the sequence to get $f(t)$. Of course, we can still compute the terms of the sequence sequentially but this will be a more long-winded process. A problem which is certain to manifest itself is that of loss of significant digits as the k -th derivative of $s^{2k-1} e^{-ts}$ is composed of terms with large coefficients which are alternatively positive and negative.

Zakian [259] takes $\delta_n(t, u)$ to be an approximation to the scaled delta function $\delta((\lambda/t) - 1)$ which is defined by

$$\int_0^T \delta \left(\frac{\lambda}{t} - 1 \right) d\lambda = t, \quad 0 < t < T, \quad (7.10)$$

$$\delta \left(\frac{\lambda}{t} - 1 \right) = 0, \quad t \neq \lambda. \quad (7.11)$$

If $f(t)$ is a continuous function it satisfies

$$f(t) = \frac{1}{t} \int_0^T \bar{f}(\lambda) \delta \left(\frac{\lambda}{t} - 1 \right) d\lambda, \quad 0 < t < T. \quad (7.12)$$

Zakian asserts that $\delta((\lambda/t) - 1)$ can be expanded into the series

$$\delta \left(\frac{\lambda}{t} - 1 \right) = \sum_{i=1}^{\infty} K_i e^{-\alpha_i \lambda/t}, \quad (7.13)$$

and his $\delta_n(t, u)$ corresponds to the first n terms of the series in (7.13). The reader can consult subsequent papers [260] and [265] to find out how the quantities K_i and α_i were computed.

7.3 Inversion of Two-dimensional Transforms

Valkó and Abate [238] have extended their approach to multi-precision inversion of Laplace transforms in one variable — see Abate and Valkó [2] — to obtain two methods for the inversion of 2-dimensional Laplace transforms. Both these methods can be considered as the concatenation of two one-dimensional methods.

The Gaver-Rho fixed Talbot method

Suppose that we are given a two-dimensional transform $\bar{f}(s_1, s_2)$ and we want to determine the original function f at (t_1, t_2) . Then, as our first step, we invert the “ s_2 ” variable to get

$$\bar{f}(s_1, t_2) = \mathcal{L}^{-1}\{\bar{f}(s_1, s_2)\}. \quad (7.14)$$

Our next step is to invert the “ s_1 ” variable to obtain

$$f(t_1, t_2) = \mathcal{L}^{-1}\{\bar{f}(s_1, t_2)\}. \quad (7.15)$$

Valkó and Abate accomplish the inversion of (7.15) by using the Gaver algorithm accelerated by the ρ -algorithm for given t_1 , t_2 and a sequence of s_1 values. Note that, for each s_1 value to be computed, we require the numerical inversion of the s_2 variable which is defined by (7.14) and this is achieved by means of the fixed Talbot algorithm (see Chapter 6). Valkó and Abate give a Mathematica program in their paper (called L2DGWRFT).

The Gaver-Rho² method

The construction of this method is the same as the Gaver-Rho fixed Talbot method except that the inner loop is also evaluated by the Gaver-Rho algorithm. A Mathematica program, called L2DGWRGWR, is also given by Valkó and Abate.

Chapter 8

The Method of Regularization

8.1 Introduction

The equation

$$\bar{f}(s) = \int_0^{\infty} e^{-st} f(t) dt, \quad (8.1)$$

is an example of a Fredholm integral equation of the first kind and another way of looking at the problem of finding $\mathcal{L}^{-1}\{\bar{f}(s)\}$ is to use a technique for solving this type of integral equation. The problems associated with solving equations of this type can be seen from the following example considered by Fox and Goodwin [87], namely,

$$\int_0^1 (x+y)\phi(y)dy = g(x). \quad (8.2)$$

For a solution to be possible the right hand side must be of the form $g(x) = a + bx$. Suppose

$$g(x) = x.$$

Fox and Goodwin note that a solution of the integral equation is

$$\phi_1(x) = 4 - 6x,$$

and, by substitution, this is clearly seen to satisfy (8.2). Unfortunately, this solution is not unique as

$$\phi_2(x) = 3 - 6x^2,$$

also satisfies (8.2) and so does every linear combination of the form

$$\alpha\phi_1(x) + (1 - \alpha)\phi_2(x).$$

Additionally, if $\psi(x)$ is any other function of x which is linearly independent of $\phi_1(x)$ and $\phi_2(x)$ and which satisfies

$$\int_0^1 (x+y)\psi(y)dy = 0,$$

then

$$\alpha\phi_1(x) + (1-\alpha)\phi_2(x) + \beta\psi(x),$$

is also a solution of the integral equation (8.2). Note that there are an infinity of such functions $\psi(x)$ as all we require is that $\psi(x)$ is orthogonal to the functions 1 and x over $[0, 1]$.

The situation is a little different with Laplace transform inversion as we have already shown that if $f(t)$ is a continuous function then its transform is unique. We recall here that there could be instability, as mentioned in Chapter 2, if $f(t)$ is not a smooth function. However, there is no reason why the methods applicable for this type of integral equation should not carry over to the case of Laplace inversion and we proceed here to give the method of regularization after giving some basic theory relating to Fredholm equations of the first kind.

8.2 Fredholm equations of the first kind — theoretical considerations

The linear Fredholm equation of the first kind is defined by

$$\int_a^b K(x, y)\phi(y)dy = g(x), \quad c \leq x \leq d, \quad (8.3)$$

or in operator form

$$\mathbf{K}\Phi = \mathbf{g}, \quad (8.4)$$

where $K(x, y)$ is the kernel of the integral equation, $\phi(x)$ is the function we would like to determine and $g(x)$ is a given function in a range (c, d) , which is not necessarily identical with the range of integration (a, b) . As noted in the previous section $g(x)$ must be compatible with the kernel $K(x, y)$. Also, if there are an infinity of solutions of $\mathbf{K}\Phi = 0$, there cannot be a unique solution of (8.3). From a numerical standpoint the worrying feature is that a small perturbation in g can result in an arbitrarily large perturbation in ϕ even if a unique solution of the integral equation exists. For if

$$h_\omega(x) = \int_a^b K(x, y) \cos \omega y \, dy, \quad c \leq x \leq d,$$

it follows from the Riemann-Lebesgue lemma that, as $\omega \rightarrow \infty$, we have $h_\omega(x) \rightarrow 0$. Thus for ω sufficiently large $h_\omega(x)$ will be arbitrarily small and if added to g will cause a change of $\cos \omega y$ in ϕ , i.e., a change which can be of

magnitude 1.

Given an integral equation of the form

$$\int_{-a}^a K(x, y)\phi(y)dy = g(x), \quad (8.5)$$

where the kernel K is symmetric, i.e. $K(x, y) = K(y, x)$ then from the Hilbert-Schmidt theory of integral equations there exists eigenfunctions $\phi_n(y)$ which satisfy the equation

$$\int_{-a}^a K(x, y)\phi_n(y)dy = \lambda_n\phi_n(x), \quad (8.6)$$

and form a complete orthonormal basis over $[-a, a]$ and the eigenvalues λ_n are real. Thus we can expand $g(x)$ in the form

$$g(x) = \sum_{n=0}^{\infty} \beta_n \phi_n(x), \quad (8.7)$$

where

$$\beta_n = \int_{-a}^a g(x)\phi_n(x)dx. \quad (8.8)$$

Since, also, we may expand $\phi(y)$ in the form

$$\phi(y) = \sum_{n=0}^{\infty} \alpha_n \phi_n(y), \quad (8.9)$$

where

$$\alpha_n = \int_{-a}^a \phi(y)\phi_n(y)dy. \quad (8.10)$$

Substitution into (8.5) gives

$$\beta_n = \lambda_n \alpha_n, \quad \text{all } n, \quad (8.11)$$

and thus we have

$$\phi(y) = \sum_{n=0}^{\infty} \frac{\beta_n}{\lambda_n} \phi_n(y). \quad (8.12)$$

The big difficulty relating to the above theory is how to compute the eigenfunctions and eigenvalues. It is apposite here to consider an example of McWhirter and Pike [154] which was concerned with the passage of light from a one-dimensional space-limited object described by the object function $O(y)$, $|y| \leq Y/2$, through a lens of finite aperture to form a band-limited image $I(x)$ which is given by the equation

$$I(x) = \frac{1}{2\pi} \int_{-\Omega}^{\Omega} d\omega e^{-i\omega x} \int_{-Y/2}^{Y/2} e^{i\omega y} O(y) dy, \quad (8.13)$$

i.e.

$$I(x) = \int_{-Y/2}^{Y/2} \frac{\sin[\Omega(y-x)]}{\pi(y-x)} O(y) dy, \quad (8.14)$$

where Ω is the highest spatial frequency transmitted by the lens. Given $I(x)$ it should in theory be possible to determine the object function $O(y)$ from which it was obtained. Practically this is not possible because a lens with finite spatial frequency Ω has an associated resolution limit π/Ω which means that an object of spatial extent Y can contain only a finite number $S = Y\Omega/\pi$ of independent components or degrees of freedom — S is known as the Shannon number in information theory. Relating this to the eigenfunction expansion (8.12) it means that the terms for which $n > Y\Omega/\pi$ must be divided by an extremely small number and so error in the value of α_n will cause these terms to diverge. Therefore these later terms must be omitted in order to get physically meaningful results.

8.3 The method of Regularization

In this method it is assumed that a solution exists to the ill-posed problem (in operator form)

$$\mathbf{K}\Phi = \mathbf{g}, \quad (8.15)$$

where now

$$\mathbf{K}\Phi \equiv \int_0^\infty e^{-st} f(t) dt,$$

and $\mathbf{g} \equiv \bar{f}(s)$, $\Re s > \gamma$. The method of determining $f(t)$ is to minimize the quadratic functional

$$\|\mathbf{K}\Phi - \mathbf{g}\| + \alpha \|\mathbf{L}\Phi\|, \quad (8.16)$$

where $\|\mathbf{L}\Phi\|$ is some linear operator and $\|\cdot\|$ denotes some appropriate norm. This minimization problem is well-posed and has a unique solution for a value of α which must be determined. Lewis [129] found that best numerical results for solving the equation (8.3) were obtained using the *zero-order regularization method* of Bakushinskii [11]. In relation to (8.3) the method consists of solving the more stable Fredholm equation of the second kind

$$\alpha\phi(x) + \int_0^1 K(x, y)\phi(y)dy = g(x), \quad (8.17)$$

when K is symmetric, i.e. $K(x, y) = K(y, x)$. In the event that $K(x, y)$ is not symmetric we form the symmetric kernel $K^*(x, y)$ where

$$K^*(x, y) = \int_c^d K(\theta, x)K(\theta, y)d\theta \quad (8.18)$$

and solve instead the integral equation

$$\alpha\phi(x) + \int_c^d K^*(x, y)\phi(y)dy = G(x), \quad (8.19)$$

where

$$G(x) = \int_c^d K(\theta, x)f(\theta)d\theta.$$

We illustrate the method by applying it to the solution of the integral equation (8.2). We form

$$\alpha\phi(x) + \int_0^1 (x+y)\phi(y)dy = x, \quad 0 \leq x \leq 1. \quad (8.20)$$

for various values of α — see Churchhouse [37]. The integral in (8.7) can be approximated by the trapezium rule so that for given x and α and step-length h , where $nh = 1$, we have

$$\alpha\phi(x) + \frac{1}{2}h \sum_{i=0}^{n-1} \{(x+ih)\phi(ih) + (x+[i+1]h)\phi([i+1]h)\} = x.$$

Setting $x = 0, h, \dots, nh$, in turn, we obtain a system of $n+1$ simultaneous linear equations in the $n+1$ unknowns $\phi(0), \phi(h), \dots, \phi(nh)$, namely

$$\alpha\phi(rh) + \frac{1}{2}h^2 \sum_{i=0}^{n-1} \{(r+i)\phi(ih) + (r+i+1)\phi([i+1]h)\} = rh, \quad r = 0, 1, \dots, n.$$

The solution of these equations is given in Table 8.1 for various α and $h = 0.1$.

It can be seen that the results tend to $\phi(x) = 4 - 6x$ as α decreases and, for a range of values of α are fairly consistent. When α is decreased further the estimated values of $\phi(x)$ diverge from $4 - 6x$. This is a characteristic feature of the method.

8.4 Application to Laplace Transforms

Suppose that in equation (8.1) we make the substitution

$$u = e^{-t},$$

then we will have transformed the integral into one over a finite range, namely

$$\bar{f}(s) = \int_0^1 u^{s-1} f(-\ln u) du, \quad (8.21)$$

or, writing $g(u) = f(-\ln u)$, we have

$$\bar{f}(s) = \int_0^1 u^{s-1} g(u) du. \quad (8.21')$$

α	$\tilde{\phi}(0)$	$\tilde{\phi}(\frac{1}{2})$	$\tilde{\phi}(1)$
2^{-4}	18.01681	2.89076	-12.23529
2^{-5}	6.34789	1.31458	-3.71873
2^{-6}	4.84588	1.11654	-2.61280
2^{-7}	4.34352	1.05144	-2.24064
2^{-8}	4.13180	1.02428	-2.08324
2^{-9}	4.03405	1.01181	-2.01044
2^{-10}	3.98703	1.00582	-1.97538
\dots	\dots	\dots	\dots
2^{-19}	3.94126	1.00001	-1.94124
2^{-20}	3.94122	1.00001	-1.94121
2^{-21}	3.94120	1.00000	-1.94119
2^{-22}	3.94119	1.00000	-1.94118
2^{-23}	3.94118	1.00000	-1.94118

Table 8.1: Solution of $\int_0^1 (x+y)\phi(x) = x$ by regularization.

If we employ a Gauss-Legendre quadrature formula with N points to evaluate this integral we obtain

$$\bar{f}(s) = \sum_{i=1}^N \alpha_i u_i^{s-1} g(u_i), \quad (8.22)$$

— this equation would be exact if the integrand could be expressed as a polynomial in u of degree $2N-1$ or less. If we substitute $s = 1, 2, \dots, N$ we obtain a system of N linear equations in the N unknowns $\alpha_i g(u_i)$

$$\sum_{i=1}^N \alpha_i u_i^k g(u_i) = \bar{f}(k+1), \quad k = 0, 1, \dots, N-1. \quad (8.23)$$

These equations have a unique solution as the determinant of the coefficients is the Vandermonde determinant which is non-zero as the u_i are distinct. Further, as we can determine the Christoffel numbers α_i from (11.25) — or alternatively by consulting the appropriate table in Abramowitz and Stegun [5] — we can compute the quantity $g(u_i)$ and hence $f(t)$ for $t = -\ln u_i$. Because of the structure of the coefficient matrix an efficient way of computing the solution of the equations is via polynomial interpolation — see Golub and van Loan [101]. As mentioned in an earlier chapter the inversion of the Laplace transform is an ill-conditioned problem. This manifests itself in the solution of the matrix equation (8.23) which we shall write as $A\mathbf{x} = \mathbf{b}$ where A is the $N \times N$ matrix with $a_{ij} = \alpha_i u_i^{j-1}$. Tikhonov [229], [230] tackles the solution of the ill-conditioned equations by attempting another problem, the minimization of

$$R(\mathbf{x}) = \langle A\mathbf{x} - \mathbf{b}, A\mathbf{x} - \mathbf{b} \rangle + h(\mathbf{x}), \quad (8.24)$$

where $\langle \cdot, \cdot \rangle$ denotes vector inner product and $h(\mathbf{x})$ is a function which is chosen to ensure the stability of the equation when minimizing over \mathbf{x} . Typically, $h(\mathbf{x}) = \lambda \|B\mathbf{x}\|^2$, where $\lambda > 0$ is the regularization parameter and B is the regularization operator. Note that if we were to take $h(\mathbf{x}) = 0$ we would be minimizing a quadratic form and would find the solution to be

$$A^T A \mathbf{x} = A^T \mathbf{b}.$$

The matrix of coefficients is now symmetric but may be even more ill-conditioned than the original A . If we have a priori knowledge of a vector \mathbf{c} which is a first approximation to \mathbf{x} then we can take

$$h(\mathbf{x}) = \lambda \langle \mathbf{x} - \mathbf{c}, \mathbf{x} - \mathbf{c} \rangle, \quad (8.25)$$

where $\lambda > 0$. The minimum value of \mathbf{x} is given by

$$\mathbf{x}(\lambda) = (A^T A + \lambda I)^{-1} (A^T \mathbf{b} + \lambda \mathbf{c}). \quad (8.26)$$

If λ is small then we are close to the value of $A^{-1} \mathbf{b}$ but $A^T A + \lambda I$ is still ill-conditioned. Increasing λ alleviates the ill-conditioning but decreases the accuracy of the solution. The choice of λ is very much hit-and-miss but the validity of the answers can be obtained by checking the goodness of fit

$$\| A \mathbf{x} - \mathbf{b} \|.$$

A more scientific approach is to choose a first approximation \mathbf{c} by initially using a 5-point Gaussian quadrature formula and then determining the fourth degree polynomial which passes through the points $(u_i, g(u_i))$. This polynomial can be used to get starting values of g at the abscissae of a 7-point quadrature formula. This will give \mathbf{c} . We can then use the iterative scheme

$$\begin{aligned} \mathbf{x}_0 &= \mathbf{c}, \\ \mathbf{x}_{n+1} &= (A^T A + \lambda I)^{-1} (A^T \mathbf{b} + \lambda \mathbf{x}_n), \end{aligned} \quad (8.27)$$

to determine \mathbf{x} , which will give estimates for $g(u_i)$ and, equivalently, $f(-\ln u_i)$. One snag about this approach is that because of the distribution of the zeros u_i the arguments of the function f will be bunched about $t = 0$. One way of avoiding this is to employ the result (1.5) so that in place of $\bar{f}(1)$, $\bar{f}(2)$, \dots we use the values $\bar{f}(1/a)$, $\bar{f}(2/a)$, \dots , $a > 0$ and solve the approximation formula

$$\sum_{i=1}^N \alpha_i u_i^{k-1} f(-a \ln u_i) = \frac{1}{a} \bar{f}(k/a), \quad k = 1, 2, \dots, N. \quad (8.28)$$

The arguments of the function f are now more scattered if $a > 1$ but the coefficient matrix and its inverse are the same as before and can be solved in the same way.

In the above regularization approach the integration has been carried out by

transforming the infinite integral to a finite integral and applying a Gauss-Legendre quadrature formula to estimate the finite integral. As we mentioned in Chapter 3 a more natural method of attacking the problem, especially in view of the exponential weight function, is via Laguerre polynomials and this is the approach adopted by Cunha and Viloche [54]. In the notation of their paper let $X = L_w^2(R^+)$ be the weighted Lebesgue space associated with $w(t) = e^{-t}$, $Y = L^2([c, d])$, $d > c > 0$ and $A : X \rightarrow Y$ the Laplace transform operator

$$(A\mathbf{x})(s) = \int_0^\infty e^{-st}x(t)dt = \bar{\mathbf{y}}(s). \quad (8.29)$$

Their problem was to determine $A^+\bar{\mathbf{y}}$ where A^+ is the generalized inverse of A and they were particularly interested in the case where $\bar{\mathbf{y}}$ is not known explicitly and we only have available perturbed data $\bar{\mathbf{y}}_\delta$ satisfying

$$\|\bar{\mathbf{y}} - \bar{\mathbf{y}}_\delta\| < \delta. \quad (8.30)$$

Cunha and Viloche employ the implicit successive approximation method of King and Chillingworth [121]

$$\mathbf{x}^{(k)} = (\lambda I + A^*A)^{-1}(\lambda\mathbf{x}^{(k-1)} + A^*\mathbf{y}_\delta), \quad \lambda > 0, \quad (8.31)$$

where A^* is the adjoint operator of A which is defined in this case by

$$(A^*v)(t) = e^t \int_c^d e^{-ts}v(s)ds,$$

— the above numbered equation should be compared to (8.27). If $L_i(t)$ denotes the Laguerre polynomial of degree i which satisfies

$$\int_0^\infty e^{-t}L_i(t)L_j(t)dt = (i!j!)\delta_{ij},$$

where $\delta_{ij} = 0$, $i \neq j$ and $\delta_{ii} = 1$, and we define the approximation

$$\mathbf{x}_N = \sum_{i=1}^N a_i L_i(t),$$

with the property that

$$\langle (\lambda I + A_N^*A_N)\mathbf{x}_N^{(k+1)}, L_j \rangle = \langle \lambda\mathbf{x}_N^{(k)} + A_N^*\bar{\mathbf{y}}_\delta, L_j \rangle, \quad j = 0, \dots, N, \quad \lambda > 0,$$

where $\langle \cdot, \cdot \rangle$ denotes inner product in X . Using the fact that

$$\bar{L}_i(s) = \frac{1}{s} \left(1 - \frac{1}{s}\right)^i$$

we can construct the matrix M whose elements M_{ij} are given by

$$M_{ij} = \int_c^d \bar{L}_i(s)\bar{L}_j(s)ds = \frac{\hat{d}^k - \hat{c}^k}{k},$$

where $\hat{d} = 1 - 1/d$, $\hat{c} = 1 - 1/c$ and $k = i + j + 1$. Next define a vector \mathbf{f} whose components are

$$f_i = \int_c^d y_\delta(s) \bar{L}_i(s) ds.$$

Then the variational formulation of the implicit scheme (8.31) will be

$$(\lambda I + M)\mathbf{a}^{(k)} = \lambda \mathbf{a}^{(k-1)} + \mathbf{f}. \quad (8.32)$$

For a given $\lambda > 0$ Cunha and Viloche give the following procedure for finding the solution:-

1. Do the Cholesky decomposition $LL^T = M + \lambda I$ — see Golub and van Loan [101].
2. Set $\mathbf{a}^{(0)} = \mathbf{0}$ and solve the system $LL^T \mathbf{a}^{(k)} = \lambda \mathbf{a}^{(k-1)} + \mathbf{f}$, $k = 1, 2, \dots$.

They point out that regularization is an important feature of the process and increasing the value of N makes the condition number of M very large. They quote a figure of $O(10^{19})$ when $N = 15$. Their paper gives an error bound estimate and the results of some numerical experiments with “noisy” data.

Hanke and Hansen [109] have given a survey of regularization methods for large scale problems and Hansen [110] presents a package consisting of 54 Matlab routines for analysis and solution of discrete ill-posed problems many of which, like Laplace inversion, arise in connection with the discretization of Fredholm integral equations of the first kind. These can be downloaded from www.netlib.org/numeralgo/na4. The website of Reichel [194] contains a substantial amount of material about recent developments in the field of regularization. One of these developments is that of multi-parameters where the minimization function takes the form

$$k \left(\|A\mathbf{x} - \mathbf{b}\|^2 + \sum_{i=1}^k \lambda_i \|B_i \mathbf{x}\|^2 \right),$$

where $k \geq 2$ and $\lambda_i > 0$, $i = 1, \dots, k$ are regularization parameters and B_i are regularization operators. See, for example, Brezinski et al [27].

Chapter 9

Survey Results

9.1 Cost's Survey

The earliest survey of numerical methods for the evaluation of Laplace transforms is probably that of Cost [49]. This listed several methods which were essentially special cases of the Post-Widder formula and the series expansion methods of Papoulis and Lanczos in terms of Legendre, Chebyshev and Laguerre polynomials, discussed in Chapter 3. Additionally, he gives a least squares formulation suggested by Schapery [205] (and independently by Rizzo and Shippy [196]) which assumes that $f(t)$ has an expansion of the form

$$f(t) = A + Bt + \sum_{k=1}^n a_k e^{-b_k t},$$

where the exponents b_k are chosen to suit the expected form of the function. The Laplace transform is

$$\bar{f}(s) = \frac{A}{s} + \frac{B}{s^2} + \sum_{k=1}^n \frac{a_k}{s + b_k},$$

so that

$$B = \lim_{s \rightarrow 0} s^2 \bar{f}(s).$$

The a_k and A can be found by assigning appropriate values to s — the values b_k and one other value are suggested — and solving a system of linear equations. Cost applies these methods to two engineering problems and draws several conclusions, some of which are a little dubious as the exact solutions to the two problems are not known. He does make the very valid point that methods such as those of Papoulis and Lanczos have a serious drawback as they require the evaluation of $\bar{f}(s)$ at prescribed values of s which may not be readily available. Piessens [181] and Piessens and Dang [184] provide bibliographies of relevant material published prior to 1975 on numerical methods and their applications

and theoretical results. At an early stage, in view of the vast amount of references one can download from the World Wide Web, this author abandoned the idea of including all material which applied numerical methods to find inverse Laplace Transforms and only a selection of the more important methods are given in the Bibliography. However a comprehensive list compiled by Volká and Vojta can be found at the website [239].

9.2 The Survey by Davies and Martin

Perhaps the most comprehensive survey available is that of Davies and Martin [60]. They take a set of 16 test functions $\tilde{f}_i(s)$, $i = 1, 2, \dots, 16$ with known inverse transforms $f_i(t)$ which were selected to reflect a variety of function types. For example, some functions are continuous and have the property that $\tilde{f}(s) \rightarrow s^\alpha$ as $s \rightarrow \infty$. Others are continuous but there is no value α for which $\tilde{f}(s) \rightarrow s^\alpha$ as $s \rightarrow \infty$ whilst other functions have discontinuities (see Table 10.1). In order to assess the accuracy of their numerical solutions they presented two measures:-

$$(i) \quad L = \left(\sum_{i=1}^{30} (f(i/2) - \hat{f}(i/2))^2 / 30 \right)^{1/2}, \quad (9.1)$$

$$(ii) \quad L' = \left(\sum_{i=1}^{30} (f(i/2) - \hat{f}(i/2))^2 e^{-i/2} / \left(\sum_{i=1}^{30} e^{-i/2} \right) \right)^{1/2}. \quad (9.2)$$

where $\hat{f}(t)$ denotes the computed value of $f(t)$. L gives the root-mean square deviation between the analytical and numerical solutions for the t values 0.5, 1, 1.5, \dots , 15 while L' is a similar quantity but weighted by the factor e^{-t} . Davies and Martin point out that L gives a fair indication of the success of a method for large t and L' for relatively small t .

Davies and Martin divide up the methods they investigated into 6 groups

- (i) Methods which compute a Sample.

These are methods which have been mentioned in Chapter 7 and which were available at that time. Of the methods chosen for comparison only the Post-Widder formula with $n = 1$ and the Gaver-Stehfest method were included from this group.

- (ii) Methods which expand $f(t)$ in Exponential Functions.

These are methods which we have included in this book under methods of Series Expansion, e.g. the methods of Papoulis of expansion in terms of Legendre polynomials and trigonometric sums. They also include in this section the method of Schapery (given above) and the method of Bellman, Kalaba and Lockett [16] which involves using the Gauss-Legendre

quadrature rule but can be regarded as a special case of the Legendre method.

(iii) Gaussian Numerical Quadrature of the Inversion Integral.

The two methods included in this section are the methods of Piessens [178] and Schmittroth (see §4.1).

(iv) Methods which use a Bilinear Transformation of s .

In this category Davies and Martin include the methods of Weeks, Piessens and Branders and the Chebyshev method due to Piessens [179] — see Chapter 3.

(v) Representation by Fourier Series.

The methods included in this group are those of Dubner and Abate, Silverberg/ Durbin and Crump — see §4.4.

(vi) Padé Approximation.

No methods were given in this category because a knowledge of the Taylor expansion about the origin might not be available. Also, Longman [139] has reported the erratic performance of this method, even with functions of the same form, but differing in some parameter value.

Davies and Martin adopt a general procedure for determining the optimum values of the variable parameters. If the paper describing the method specifies an optimum value of a parameter under certain conditions, that value is adopted if appropriate. For example, Crump [53] noted that $T = 0.8t_{\max}$ gives fairly optimal results. For the remaining parameters a reasonable spread of parameter values was used in preliminary tests and, assuming that best results on most of the test functions were obtained in a small range of parameter values, final tests were made covering these values more closely. “Optimum” parameter values for any given test function are taken to be the ones that give the highest accuracy with respect to the measures L and L' . They also devise a scheme for getting “optimum” parameter values based on optimum parameter values for the 32 measures of best fit (a value of L and L' for each test function).

As a general rule of guidance Davies and Martin advocate the use of more than one numerical inversion method especially when dealing with an unknown function. Their overall conclusion, on the basis of the 16 functions tested, was that the Post-Widder method in group (i), i.e. with $n = 1$, and all the methods in group (ii) seldom gave high accuracy. The Gaver-Stehfest method, however, gave good accuracy over a fairly wide range of functions. They report that the methods in group (iv) give exceptional accuracy over a wide range of functions as does the method of Crump from group (v). The other Fourier series methods and the methods in group (iii) gave good accuracy on a fairly wide range of functions.

Where special situations apply other methods might be more appropriate. Thus if $\bar{f}(s)$ is a rational function the method of Padé approximation gives highly accurate results. Again, if $\bar{f}(s)$ is known only on the real axis, or the determination of $\bar{f}(s)$ for complex s is very difficult, then the Chebyshev method of Piessens

and the Gaver-Stehfest method are to be preferred (in that order). Note that values of t considered by Davies and Martin satisfied $t \leq 15$.

9.3 Later Surveys

9.3.1 Narayanan and Beskos

Narayanan and Beskos [160] compare eight methods of Laplace transform inversion. They can be grouped into three categories:-

- (i) Interpolation — collocation methods;
- (ii) Methods based on expansion in orthogonal functions;
- (iii) Methods based on the Fourier transform.

In the first group they describe what they call ‘Method of maximum degree of precision’, which is essentially the method of Salzer given in Chapter 4 as extended by Piessens. They remark that extensive tables of the relevant quadrature formulae are given in Krylov and Skoblya [122]. The second method in this group was Schapery’s collocation method (see §9.1) and the third method was the Multidata method of Cost and Becker [50]. The latter method assumes that

$$f(t) = \sum_{i=1}^n a_i e^{-b_i t}, \quad (9.3)$$

and by minimizing the mean square error in the above approximation they obtain the system of equations

$$\sum_{j=1}^m s_j f(s_j) \left[1 + \frac{b_k}{s_j}\right]^{-1} = \sum_{j=1}^m \sum_{i=1}^n a_i \left[1 + \frac{b_i}{s_j}\right]^{-1} \left[1 + \frac{b_k}{s_j}\right] \quad k = 1, 2, \dots, n \quad (9.4)$$

By pre-selecting the sequence $\{b_i\}$ equation (9.4) represents a system of linear equations from which the a_i can be determined. However, the big problem is in the selection of good values of the b_i .

In the second group of methods Narayanan and Beskos include the method of Papoulis where they assume that the function $f(t)$ is expressible as a sine series, the expansion of $f(t)$ in terms of Legendre polynomials and Weeks’s method of inversion using Laguerre polynomials. In this latter method they mention that the coefficients in the expansion can be computed efficiently by using the Fast Fourier Transform as demonstrated by Wing [256].

In the final group they give the methods of Cooley, Lewis and Welch [46] and Durbin [73].

Their conclusions about the relative efficacy of the various methods was that the interpolation method of Salzer/Piessens, the Weeks method and the two methods from group (iii) provide very good results (within plotting accuracy) while the remaining four are generally very poor.

9.3.2 Duffy

Duffy [72] used the survey by Davies and Martin as the background for his paper on the Comparison of Three New Methods on the Numerical Inversion of Laplace Transforms. Two of the methods had been known to Davies and Martin, namely those of Weeks and Crump, but had been considerably improved by Lyness and Giunta [150] and Honig and Hirdes [112] respectively after the survey — the method of Talbot was not known to them at the time. Murli and Rizzardi [159] give an algorithm for Talbot's method and Garbow et al [92] have given an algorithm for the improved Weeks method while Honig and Hirdes give their own Fortran program. Duffy, in addition to using the 16 test functions in Davies and Martin, concentrates his tests on three types of transforms:- those that have only poles, those with a mixture of poles and branch points and those having only branch points. He also looked at the inversion of joint Fourier-Laplace transforms.

Duffy reports very good results for Talbot's method with the exception of Test 1 (the Bessel function $J_0(t)$). Talbot [226] mentions that the presence of branch points can cause problems and gives a strategy for overcoming this and obtained results which were on a par with those obtained for other functions (Other authors have obtained good results by computing $1/\sqrt{s^2+1}$ as $1/[\sqrt{s+i}\sqrt{s-i}]$). Talbot's method was not applicable to Test 12 because that transform had an infinity of poles on $\Re s = 0$. Poor results were also obtained for this Test function by the other two methods. The Honig and Hirdes method was also fairly poor when the function $f(t)$ had a discontinuity as in Test 10. The Garbow et al method also encountered difficulties when the function $f(t)$ possessed a singularity at the origin of the form \sqrt{t} or $\ln t$.

9.3.3 D'Amore, Laccetti and Murli

D'Amore et al [56] also compared several methods with their own routine INVLTF. In particular the NAG routine C06LAF which is based on the method of Crump, the NAG routines C06LBF and C06LCF which are based on the Garbow et al method, the routine DLAINV which is given as Algorithm 619 in the ACM Collected Algorithms and the routine LAPIN of Honig and Hirdes. They concentrated their attention on eight test functions $\bar{f}_1(s)$, $\bar{f}_{10}(s)$, $\bar{f}_{15}(s)$, $\bar{f}_{18}(s)$, $\bar{f}_{28}(s)$, $\bar{f}_{30}(s)$, $\bar{f}_{32}(s)$, $\bar{f}_{34}(s)$ (see list of Test Transforms). d'Amore et al carry out their investigations for two sets of values of t , $t \in [1, 15.5]$ (t small) and $t \in [15.5, 100]$ (t large). The parameters in the routines were taken to be the default parameters and an accuracy of 10^{-7} was requested for each package. Double precision arithmetic was used throughout. The program C06LBF was not tested on the functions $\bar{f}_{10}(s)$ and $\bar{f}_{34}(s)$ as the Weeks method requires the continuity of the inverse Laplace transform.

d'Amore et al assert that LAPIN is not an automatic routine so that comparisons can only be made in general terms. They estimate that INVLTF is faster than LAPIN by factors of 6 or 7. With regard to DLAINV they feel that IN-

VLTF works much better in terms of function evaluation and put this down to a better discretization estimate. The NAG routines were more efficient if the inverse transform had to be computed for a range of values of t . However, their performance depended heavily on the choice of their incidental parameters. This was particularly the case when the error indicator suggested that the program be re-run with a new choice of parameters. They reported that the routine C06LAF returned no result for $t = 5.5$ for the function f_1 and for several values of t for f_{34} . In all these routines it was particularly important to get a correct value of c which is an upper bound for γ . If one chooses c less than γ the routine might appear to work well but will, in general, produce a completely erroneous result.

9.3.4 Cohen

The present author has used the programs given at the URL www.cf.ac.uk/maths/cohen/programs/inverselaplace/transform/ to compare the methods of Crump, Gaver/Post-Widder, Honig-Hirdes, Sidi, Talbot and Weeks. The comparison is in some ways unfair as some of the methods use double precision arithmetic (approximately 16 decimal digits) while others use quadruple precision arithmetic and the program for Talbot's method is essentially single length. Ideally, to minimize errors due to severe cancellation, quadruple precision arithmetic would be desirable in all cases. Higher precision still would be advantageous as has been shown by Abate and Valkó [2] in a recent paper. However, for the benefit of users, it was decided at an early stage to include some tested routines in case newer routines failed. It should be noted that all the methods are critically dependent on parameters and a poor selection of these parameters will yield unsatisfactory results. It is thus recommended that as many methods as possible are tried in order to get a consensus value and, wherever possible, programs should be rerun using different (but sensible) parameters.

In the table at the end of this chapter there is a list of 34 test transforms which have been used by other investigators. For the comparisons we have decided to select the following test transforms $\bar{f}_1(s)$, $\bar{f}_3(s)$, $\bar{f}_{11}(s)$, $\bar{f}_{15}(s)$, $\bar{f}_{25}(s)$, $\bar{f}_{30}(s)$, $\bar{f}_{34}(s)$ together with the additional transform $\bar{f}_{35}(s)$. This latter function exhibits additional properties which are not present in the previous members of the list because of the combination of fractional powers of s in the denominator. We have omitted $\bar{f}_{10}(s)$ from the list of examples chosen by d'Amore et al as this is a particular example of a transform which can be easily found by considering $g(s) = 1/s$ and then applying the translation theorem. Another useful device which can be effective in extending the range of values for which a method is successful is to apply the shift theorem. Thus instead of computing $f(t)$ we compute $g(t)$ where $g(s) = f(s + \alpha)$, for suitable α . It then follows that $f(t) = e^{\alpha t}g(t)$. This was particularly useful in the case of $\bar{f}_{30}(s)$. The calculations have been carried out for a selection of values of t , namely, $t_k = 2^{k-1}$, $k = 0, 1, \dots, 7$. These computations were performed on the Thor UNIX computer at Cardiff University.

t	$f_1(t)$	$f_3(t)$	$f_{11}(t)$	$f_{15}(t)$
0.5	0.9384698072	0.7788007831	0.1159315157	1.070641806 ^[-3]
1.0	0.7651976866	0.6065306597	-0.5772156649	2.066698535 ^[-2]
2.0	0.2238907791	0.3678794412	-1.2703628455	5.399096651 ^[-2]
4.0	-0.3971498099	0.1353352832	-1.9635100260	5.188843718 ^[-2]
8.0	0.1716508071	1.831563889 ^[-2]	-2.6566572066	3.024634056 ^[-2]
16.0	-0.1748990740	3.354626279 ^[-4]	-3.3498043871	1.373097780 ^[-2]
32.0	0.1380790097	1.125351747 ^[-7]	-4.0429515677	5.501020731 ^[-3]
64.0	9.259001222 ^[-2]	1.266416555 ^[-14]	-4.7360987483	2.070340096 ^[-3]

Table 9.1: Numerical values of test functions

t	$f_{25}(t)$	$f_{30}(t)$	$f_{34}(t)$	$f_{35}(t)$
0.5	0.7978845608	0.1270895400	0	0.3567230473
1.0	1.1283791671	0.5682668420	0.5	0.2356817540
2.0	1.5957691216	4.5667335568	0.5	0.1551649316
4.0	2.2567583342	2.484103565 ^[2]	0.5	0.1018061471
8.0	3.1915382432	7.405092100 ^[5]	0.5	6.657603724 ^[-2]
16.0	4.5135166684	6.580246682 ^[12]	0.5	4.339956704 ^[-2]
32.0	6.3830764864	5.195957567 ^[26]	0.5	2.820616527 ^[-2]
64.0	9.0270333368	3.239757005 ^[54]	0.5	1.827963282 ^[-2]

Table 9.2: Numerical values of test functions

In the first two tables 9.1, 9.2 we present the correct values, to 10 places of decimals/10 significant digits, of $f_k(t)$ for the functions we have selected. In the next tables we give an indication of the number of correct decimal digits/significant digits obtained by employing the various methods outlined above. Some results were obtained to more than 10 decimal places/significant digits and where this has occurred we have written 10 in bold form — in some of these cases more than 20 decimal digit accuracy was obtained. An asterisk indicates that the method was not applicable to the given transform as, for example, Weeks's method for $f_{11}(t)$. A question mark indicates that no results were printed for those t -values. In the case of the author's variation of the Sidi method, §4.3, it sometimes happens that A and B do not agree to 10 decimal places and where this occurs we have selected the quantity which gives the most accurate answer (by assessing the behaviour of the terms in the respective algorithm). Selection has been indicated by a dagger. In addition to the Fortran programs we have included the Mathematica program of Abate and Valkó [2] for Talbot's method which gives excellent results when the parameters are chosen appropriately.

For the function $\bar{f}_1(s)$ most methods, with the exception of Talbot where the results of Duffy were replicated when $\bar{f}(s)$ was set at $1/\sqrt{s^2 + 1}$, gave reasonable answers (5 decimal place accuracy was requested for the Crump and

t	C	G/P-W	H-H	S	T	W
0.5	5	10	10	10 †	4	5
1.0	5	10	10	10	5	5
2.0	5	10	10	10	5	5
4.0	5	8	10	10	2	5
8.0	5	4	10	10	3	5
16.0	4	4	10	10	3	4
32.0	5	?	10	10	4	0
64.0	5	?	0	6	3	0

Table 9.3: Comparison of methods for $f_1(t)$

t	C	G/P-W	H-H	S	T	W
0.5	3	10	10	10	4	5
1.0	3	10	10	10	7	5
2.0	3	10	10	10	6	5
4.0	5	10	10	10	5	5
8.0	5	10	10	10	3	4
16.0	1?	10	10	10	2	1
32.0	?	10	10	10	0	0
64.0	?	?	6	10	0	0

Table 9.4: Comparison of methods for $f_3(t)$

Weeks method and the formulation of the Talbot program constrains the relative accuracy to $O(10^{-6})$. Setting $\bar{f}(s) = 1/\sqrt{s+i}\sqrt{s-i}$ gave the results in the above table which are given in the Talbot column — see Abate and Valkó. For the Gaver method the ρ -algorithm did not converge for $t = 16, 32, 64$. However the $W^{(m)}$ -algorithm did converge for $t = 16$. The value $t = 64$ proved to be more than a match for all methods except the Crump and Sidi.

With regard to the function $\bar{f}_3(s)$ most methods worked well for smaller values of t . However the Crump, Talbot and Weeks methods were very poor for $t \geq 16$. The Sidi method was the only one to get good results for $t = 64$.

For the function $\bar{f}_{11}(s)$ the Weeks method was not applicable for this function. All other methods performed well.

The Gaver and Honig-Hirdes methods came out best for the function $\bar{f}_{15}(s)$ although, as mentioned in §4.3, a considerable improvement can be effected by applying the Sidi approach in complex form with suitably modified x_ℓ .

The Gaver, Honig-Hirdes, Sidi and Talbot methods worked extremely well for the function $\bar{f}_{25}(s)$.

The Sidi method out-performed all the other methods for the function $\bar{f}_{30}(s)$ while the Talbot and Weeks methods were consistently good for $t \leq 16$. The Talbot Mathematica program did get good results for these values when an

t	C	G/P-W	H-H	S	T	W
0.5	0	10	10	10	4	*
1.0	5	10	10	10	5	*
2.0	5	10	10	10	6	*
4.0	5	10	10	10	5	*
8.0	5	10	10	10	5	*
16.0	5	10	10	10	5	*
32.0	5	10	10	10	5	*
64.0	3	10	10	10 [†]	7	*

Table 9.5: Comparison of methods for $f_{11}(t)$

t	C	G/P-W	H-H	S	T	W
0.5	0	10	9	10	2	*
1.0	0	10	10	10	4	*
2.0	1	9	10	7	4	*
4.0	0	9	10	6	4	*
8.0	0	10	10	3 [†]	5	*
16.0	0	10	10	6 [†]	4	*
32.0	0	10	10	8 [†]	3	*
64.0	0	10	10	10 [†]	3	*

Table 9.6: Comparison of methods for $f_{15}(t)$

t	C	G/P-W	H-H	S	T	W
0.5	*	10	10	10	6	*
1.0	*	10	10	10	7	*
2.0	*	10	10	10	7	*
4.0	*	10	10	10	8	*
8.0	*	10	10	10	8	*
16.0	*	10	10	10	7	*
32.0	*	10	10	10	7	*
64.0	*	10	10	10	7	*

Table 9.7: Comparison of methods for $f_{25}(t)$

t	C	G/P-W	H-H	S	T	W
0.5	4	10	10	10	5	5
1.0	4	10	10	10	6	5
2.0	4	8	8	10	6	5
4.0	?	9	0	10	4	5
8.0	?	0	0	10	5	5
16.0	?	0	0	10 †	4	4
32.0	?	0	0	10 †	5	0
64.0	?	0	0	10	0	0

Table 9.8: Comparison of methods for $f_{30}(t)$

M	t	$f_{30}(t)$
300	0.5	0.127089539996054215885673481679998
	1.0	0.568266842009869230412941804595398
	2.0	4.56673355677501693150021934399341
	4.0	248.410356547740449616160896803338
	8.0	740509.209988052727930341834736775
	16.0	$6.58024668189005793008079079342660 \times 10^{12}$
	32.0	$5.19595756734301406909103225744039 \times 10^{26}$
	64.0	$-3.22412909586142947581050430394136 \times 10^{37}$
400	64.0	$3.239757004995495910185561406964565 \times 10^{54}$

Table 9.9: Mathematica results for $f_{30}(t)$ by Talbot’s method.

appropriate contour (precision control factor) was chosen. Results for this case are given in Table 9.9, where all the results are given rounded to 32 significant figures.

Results for function $\bar{f}_{34}(s)$ were very mixed. Apart from $t = 0.5$ the t -values are points of discontinuity of the function and the average value of 0.5 should be returned. The Crump method gives a zero answer for $t = 1, 2, 4$ but is accurate for all other values. For $t = 32$ the Honig-Hirdes and Sidi methods yield incorrect results. Surprisingly, values obtained for $t = 64$ were accurate. Trials suggested that this value is obtained for all values $t > t_0$, for some t_0 , and, in this range of t , we are determining the value in mean of $f_{34}(t)$. Although, technically, Talbot’s method is supposed to fail when we have an infinity of singularities on the imaginary axis some good results were obtained by using the Talbot Mathematica program but this was only because of the choice of t resulted in determining $f(t)$ at points of discontinuity.

The Gaver, Honig-Hirdes and Sidi methods worked extremely well on the function $\bar{f}_{35}(s)$. The Talbot method was consistent but did not yield the same order of accuracy — double length arithmetic would have helped here. The Mathematica program gave excellent results.

t	C	G/P-W	H-H	S	T	W
0.5	5	3	10	10 †	*	*
1.0	0	1	4	2	*	*
2.0	0	1	2	2†	*	*
4.0	0	1	1	2	*	*
8.0	5	1	2	3	*	*
16.0	5	6	5	6†	*	*
32.0	5	10	0	?	*	*
64.0	5	10	10	10	*	*

Table 9.10: Comparison of methods for $f_{34}(t)$

t	C	G/P-W	H-H	S	T	W
0.5	*	10	10	10	4	*
1.0	*	10	10	10	5	*
2.0	*	10	10	10	5	*
4.0	*	10	10	10	4	*
8.0	*	10	10	10	4	*
16.0	*	10	10	10	3	*
32.0	*	10	10	10	3	*
64.0	*	10	10	10	4	*

Table 9.11: Comparison of methods for $f_{35}(t)$

9.4 Test Transforms

i	$\tilde{f}_i(s)$	$f_i(t)$
1	$(s^2 + 1)^{-1/2}$	$J_0(t)$
2	$s^{-1/2}e^{-1/s}$	$(\pi t)^{-1/2} \cos(2\sqrt{t})$
3	$(s + \frac{1}{2})^{-1}$	$e^{-t/2}$
4	$1/((s + 0.2)^2 + 1)$	$e^{-0.2t} \sin t$
5	s^{-1}	1
6	s^{-2}	t
7	$(s + 1)^{-2}$	te^{-t}
8	$(s^2 + 1)^{-1}$	$\sin t$
9	$s^{-1/2}$	$(\pi t)^{-1/2}$
10	$s^{-1}e^{-5s}$	$H(t - 5)$
11	$s^{-1} \ln s$	$-C - \ln t$
12	$(s(1 + e^{-s}))^{-1}$	$g(t) = g(2 + t), \quad g(t) = \begin{cases} 1, & 0 < t < 1 \\ 0, & 1 < t < 2 \end{cases}$
13	$(s^2 - 1)(s^2 + 1)^{-2}$	$t \cos t$
14	$(s + \frac{1}{2})^{1/2} - (s + \frac{1}{4})^{1/2}$	$(e^{-t/4} - e^{-t/2})(4\pi t^3)^{-1/2}$
15	$e^{-4s^{1/2}}$	$2e^{-4/t}(\pi t^3)^{-1/2}$
16	$\arctan(1/s)$	$t^{-1} \sin t$
17	$1/s^3$	$\frac{1}{2}t^2$
18	$1/(s^2 + s + 1)$	$(2/\sqrt{3})e^{-t/2} \sin(\sqrt{3}t/2)$
19	$3/(s^2 - 9)$	$\sinh(3t)$
20	$120/s^6$	t^5
21	$s/(s^2 + 1)^2$	$\frac{1}{2}t \sin t$
22	$(s + 1)^{-1} - (s + 1000)^{-1}$	$e^{-t} - e^{-1000t}$
23	$s/(s^2 + 1)$	$\cos t$
24	$1/(s - 0.25)^2$	$te^{t/4}$
25	$1/s\sqrt{s}$	$2\sqrt{(t/\pi)}$
26	$1/(s + 1)^{1/2}$	$e^{-t}/\sqrt{\pi t}$
27	$(s + 2)/s\sqrt{s}$	$(1 + 4t)/\sqrt{\pi t}$
28	$1/(s^2 + 1)^2$	$\frac{1}{2}(\sin t - t \cos t)$
29	$1/s(s + 1)^2$	$1 - e^{-t}(1 + t)$
30	$1/(s^3 - 8)$	$\frac{1}{12}e^{-t}[e^{3t} - \cos(\sqrt{3}t) - \sqrt{3}\sin(\sqrt{3}t)]$
31	$\ln[(s^2 + 1)/(s^2 + 4)]$	$2[\cos(2t) - \cos t]/t$
32	$\ln[(s + 1)/s]$	$(1 - e^{-t})/t$
33	$(1 - e^{-s})/s^2$	$\begin{cases} t & 0 \leq t \leq 1 \\ 1 & \text{otherwise} \end{cases}$
34	$1/[s(1 + e^s)]$	$\begin{cases} 0 & 2k < t < 2k + 1 \\ 1 & 2k + 1 < t < 2k + 2 \end{cases} \quad \forall k.$
35	$1/(s^{1/2} + s^{1/3})$	Series expansion given in §4.1

Chapter 10

Applications

10.1 Application 1. Transient solution for the Batch Service Queue $M/M^N/1$

In this application we are modelling customers arriving at random who are served in batches of maximum size N . This is exactly the situation which arises with the operation of lifts in stores or office blocks as safety considerations limit the number of people who can use the lift. It is assumed that the inter-arrival time of customers has a negative exponential distribution with mean λ and that the service time of batches has a negative exponential distribution with mean μ . The problem to be solved is the determination of the mean number of customers in the queue as a function of time — see Griffiths et al [107].

Derivation of the Model Equations.

Let $p_n(t)$ denote the probability that there are n customers in the queue at time t . Then the probability $p_0(t + \delta t)$ that there are no customers at time $t + \delta t$ equals the probability that there were no customers at time t multiplied by the probability of no new arrivals in time δt plus the sum of the probabilities of there being i ($i = 1, \dots, N$) at time t and a batch service having taken place between t and $t + \delta t$. Thus

$$p_0(t + \delta t) = p_0(t)[1 - \lambda\delta t] + \sum_{i=1}^N p_i(t)[1 - \lambda\delta t]\mu\delta t.$$

Rearranging

$$\frac{p_0(t + \delta t) - p_0(t)}{\delta t} = -\lambda p_0(t) + \sum_{i=1}^N p_i(t)[1 - \lambda\delta t]\mu,$$

and, as $\delta t \rightarrow 0$, we obtain

$$\frac{dp_0}{dt} = -\lambda p_0(t) + \mu \sum_{i=1}^N p_i(t). \quad (10.1)$$

Similarly, for $n \geq 1$ we have

$$p_n(t + \delta t) = p_n(t)[1 - \lambda\delta t][1 - \mu\delta t] + p_{n-1}(t)\lambda\delta t[1 - \mu\delta t] + p_{n+N}(t)[1 - \lambda\delta t]\mu\delta t,$$

leading to

$$\frac{dp_n}{dt} = -(\lambda + \mu)p_n(t) + \lambda p_{n-1}(t) + \mu p_{n+N}(t), \quad n \geq 1. \quad (10.2)$$

We now solve the system of differential equations (10.1), (10.2).

Solution of the Model Equations.

Let

$$G(z, t) = \sum_{n=0}^{\infty} z^n p_n(t), \quad (10.3)$$

be the probability generating function associated with the model. Then from (10.1), (10.2) we have

$$\begin{aligned} \frac{dp_0}{dt} &= -\lambda p_0(t) + \mu[p_1(t) + p_2(t) + \cdots + p_N(t)], \\ z \frac{dp_1}{dt} &= -(\lambda + \mu)z p_1(t) + \lambda z p_0(t) + \mu z p_{N+1}(t), \\ z^2 \frac{dp_2}{dt} &= -(\lambda + \mu)z^2 p_2(t) + \lambda z^2 p_1(t) + \mu z^2 p_{N+2}(t), \\ &\vdots \end{aligned}$$

Summation by columns gives

$$\begin{aligned} \frac{\partial G(z, t)}{\partial t} &= -(\lambda + \mu)[G(z, t) - p_0(t)] + \lambda z G(z, t) + \frac{\mu}{z^N} [G(z, t) - \sum_{i=0}^N z^i p_i(t)] \\ &\quad - \lambda p_0(t) + \mu \sum_{i=1}^N p_i(t), \end{aligned}$$

or

$$\frac{\partial G}{\partial t} = -(\lambda + \mu)G(z, t) + \lambda z G(z, t) + \frac{\mu}{z^N} G(z, t) - \frac{\mu}{z^N} \sum_{i=0}^N z^i p_i(t) + \mu \sum_{i=0}^N p_i(t),$$

which can be written as

$$\frac{\partial G}{\partial t} = [-(\lambda + \mu) + \lambda z + \frac{\mu}{z^N}]G(z, t) + \mu \sum_{i=0}^N p_i(t) - \frac{\mu}{z^N} \sum_{i=0}^N z^i p_i(t). \quad (10.4)$$

Now let $\bar{G}(z, s)$ denote the Laplace transform of $G(z, t)$ that is

$$\bar{G}(z, s) = \int_0^\infty e^{-st} G(z, t) dt, \quad (10.5)$$

then the transform of (10.4) is

$$s\bar{G}(z, s) - G(z, 0) = [-\lambda(1 - z) - \mu(1 - \frac{1}{z^N})]\bar{G}(z, s) + \mu \sum_{i=0}^N \bar{p}_i(s) - \frac{\mu}{z^N} \sum_{i=0}^N z^i \bar{p}_i(s),$$

where $\bar{p}_i(s)$ is the Laplace transform of $p_i(t)$. On the assumption that nothing is in the system at $t = 0$ we have $G(z, 0) = 1$ and consequently

$$\left[s + \lambda(1 - z) + \mu \left(1 - \frac{1}{z^N} \right) \right] \bar{G}(z, s) = 1 + \mu \sum_{i=0}^N \bar{p}_i(s) - \frac{\mu}{z^N} \sum_{i=0}^N z^i \bar{p}_i(s).$$

Equivalently,

$$\bar{G}(z, s) = \frac{z^N + \mu \sum_{i=0}^N (z^N - z^i) \bar{p}_i(s)}{[s + \lambda(1 - z)]z^N + \mu(z^N - 1)}. \quad (10.6)$$

The denominator in (10.6) is a polynomial of degree $N + 1$ in z , call it $q(z)$, where

$$q(z) = -\lambda z^{N+1} + (s + \lambda + \mu)z^N - \mu, \quad (10.7)$$

and thus has $N + 1$ zeros. Certainly, if $\mu \leq \lambda$, and $\Re s \geq \gamma$ for appropriate γ , there are exactly N zeros within the unit circle and one zero outside (see Appendix 11.6). As $\bar{G}(z, s)$ must be analytic inside and on the unit circle, the numerator must vanish at the N zeros z_1, z_2, \dots, z_N of the denominator which lie within the unit circle, i.e., we may write the numerator as

$$A(z - z_1)(z - z_2) \dots (z - z_N), \quad |z_i| < 1, \quad i \leq N,$$

where A is a constant. (10.6) becomes

$$\bar{G}(z, s) = \frac{A(z - z_1)(z - z_2) \dots (z - z_N)}{[s + \lambda(1 - z)]z^N + \mu(z^N - 1)}. \quad (10.8)$$

To determine A we note that

$$\bar{G}(1, s) = \mathcal{L}\{G(1, t)\} = \int_0^\infty e^{-st} G(1, t) dt.$$

But

$$\begin{aligned} G(1, t) &= \left[\sum_{n=0}^{\infty} z^n p_n(t) \right]_{z=1}, \\ &= \sum_{n=0}^{\infty} p_n(t) = 1, \end{aligned}$$

so that

$$\bar{G}(1, s) = \mathcal{L}\{1\} = 1/s.$$

Hence

$$\frac{1}{s} = \frac{A \prod_{i=1}^N (1 - z_i)}{s},$$

giving

$$A = \frac{1}{\prod_{i=1}^N (1 - z_i)}.$$

Substituting for A in (10.8) and observing that the denominator has the representation

$$-\lambda(z - z_1)(z - z_2) \dots (z - z_N)(z - z_{N+1}), \quad |z_{N+1}| > 1,$$

we find that

$$\bar{G}(z, s) = \frac{1}{\lambda(z_{N+1} - z) \prod_{i=1}^N (1 - z_i)}. \quad (10.9)$$

Writing $z_{N+1} - z = z_{N+1}(1 - z/z_{N+1})$ we can expand (10.9) as a power series in z . The coefficient of z^n will be $\bar{p}_n(s)$ where

$$\bar{p}_n(s) = \frac{1}{\lambda \left[\prod_{i=1}^N (1 - z_i) \right] z_{N+1}^{n+1}}. \quad (10.10)$$

$p_n(t)$ could be determined if it was possible to invert this transform (the difficulty being that z_1, \dots, z_{N+1} are all unknown functions of s).

Determination of the Mean number of Customers at time t .

Denote by $M(t)$ the mean number of customers in the queue at time t . Then

$$M(t) = \sum_{n=0}^{\infty} n p_n(t),$$

and thus, taking Laplace transforms,

$$\bar{M}(s) = \sum_{n=0}^{\infty} n \bar{p}_n(s). \quad (10.11)$$

The sum on the right hand side of (10.11) can be derived from

$$\begin{aligned} \bar{G}(z, s) &= \int_0^{\infty} e^{-st} G(z, t) dt = \int_0^{\infty} \left(\sum_0^{\infty} z^n p_n(t) \right) dt, \\ &= \sum_0^{\infty} z^n \int_0^{\infty} e^{-st} p_n(t) dt = \sum_0^{\infty} z^n \bar{p}_n(s), \end{aligned}$$

giving

$$\frac{\partial \bar{G}}{\partial z} = \sum_0^{\infty} n z^{n-1} \bar{p}_n(s),$$

and consequently

$$\bar{M}(s) = \left\{ \frac{\partial \bar{G}}{\partial z} \right\}_{z=1}. \quad (10.12)$$

Hence from (10.9)

$$\begin{aligned} \bar{M}(s) &= \frac{1}{\lambda(\prod_{i=1}^N (1 - z_i))(z_{N+1} - 1)^2}, \\ &= \frac{1}{\lambda(\prod_{i=1}^{N+1} (1 - z_i))(1 - z_{N+1})}, \\ &= \frac{-1}{s(1 - z_{N+1})}, \end{aligned} \quad (10.13)$$

as the first part of the denominator is exactly the denominator of (10.8) when $z = 1$. Recall that the formula (10.13) is only valid for $\Re s \geq \gamma$ and it would be invalid if additional zeros of the denominator of (10.6) were outside the unit circle.

Formula (10.13) is a lot simpler than formula (10.10), as it only involves one unknown z_{N+1} . But it still means that we cannot express $\bar{M}(s)$ in terms of s explicitly and this presents some difficulties in the application of some of the numerical methods for inverting the Laplace transform. We note, however,

that for a given numerical value of s the root z_{N+1} is determinable by any good root solving process from equation (10.7), which enables $\bar{M}(s)$ to be determined from (10.13). Care must be taken, however, to ensure that we don't infringe the condition $\Re s \geq \gamma$.

Example 10.1 Consider the case $\lambda = 3, \mu = 1, N=2$. Several approaches suggest themselves for determining $\bar{M}(s)$:-

1. Rational approximation.

z_3 now satisfies the cubic equation

$$q(z) = z^3 - \frac{1}{3}(s+4)z^2 + \frac{1}{3} = 0,$$

and a first approximation to the root is

$$z_3^{(1)} = \frac{1}{3}(s+4).$$

Consequently an approximation to $\bar{M}(s)$ is $\bar{M}_1(s)$ where, from (10.13),

$$\bar{M}_1(s) = \frac{3}{s(s+1)} = \frac{3}{s} - \frac{3}{s+1},$$

yielding the approximate solution

$$M_1(t) = 3 - 3e^{-t}.$$

A second approximation can be obtained by applying the Newton-Raphson formula

$$z_3^{(2)} = z_3^{(1)} - q(z_3^{(1)})/q'(z_3^{(1)}),$$

which yields

$$z_3^{(2)} = \frac{1}{3}(s+4) - \frac{3}{(s+4)^2},$$

giving an approximation $\bar{M}_2(s)$,

$$\bar{M}_2(s) = \frac{3(s+4)^2}{s(s^3 + 9s^2 + 24s + 7)},$$

and hence

$$M_2(t) = \frac{48}{7} - Ae^{-\alpha t} - e^{-\beta t}(B \cos \gamma t + C \sin \gamma t),$$

where

$$\begin{array}{ll} A = 6.635827218 & \alpha = 0.331314909 \\ B = 0.221315642 & \beta = 4.334342545 \\ C = 0.157806294 & \gamma = 1.530166685 \end{array}$$

s	$1/s$	$\bar{f}(s)$
2	0.500	1.100736169
4	0.250	0.6180339887
5	0.200	0.5096822474
8	0.125	0.3356892445

Table 10.1: Table of function values for Lagrange interpolation.

A further application of the Newton-Raphson formula produces

$$z_3^{(3)} = P(s)/Q(s),$$

where

$$P(s) = s^9 + 36s^8 + 576s^7 + 5331s^6 + 31176s^5 + 118224s^4 \\ + 286869s^3 + 421884s^2 + 332784s + 102286,$$

and

$$Q(s) = 3(s+4)^2(s^3 + 12s^2 + 48s + 55)(s^3 + 12s^2 + 48s + 37),$$

from which we can determine an approximation $M_3(t)$ (see Chapter 5).

2. Interpolation.

Since

$$\bar{M}(s) = -1/s(1 - z_{N+1}),$$

we have, on the assumption that $\bar{f}(s) = -1/(1 - z_{N+1})$ can be expanded as a series in $1/s$,

$$\bar{M}(s) = \frac{a_1}{s} + \frac{a_2}{s^2} + \frac{a_3}{s^3} + \cdots.$$

For appropriate choice of s we can evaluate the function $-1/(1 - z_{N+1})$ and then use the Lagrange interpolation formula to approximate $\bar{f}(s)$. Thus,

$$\bar{f}(s) \approx \sum_{i=1}^k L_i(1/s) \bar{f}(s_i), \quad (10.14)$$

where

$$L_i(1/s) = \prod_{j \neq i} \left(\frac{1}{s} - \frac{1}{s_j} \right) / \prod_{j \neq i} \left(\frac{1}{s_i} - \frac{1}{s_j} \right).$$

For the example we are considering we have computed $\bar{f}(s)$ for a number of values of s which are recorded in Table 10.1

k	$u_k = 1/s_k$	$\bar{f}(s_k)$
1	0.96194	1.85478
2	0.69134	1.42822
3	0.30866	0.73906
4	0.03806	0.11003

Table 10.2: Data for interpolation by Chebyshev polynomials.

Application of the Lagrange interpolation formula gives

$$\bar{f}(s) \approx \frac{1.1614792}{s^3} - \frac{1.8908255}{s^2} + \frac{2.84078075}{s} + 0.007867285,$$

and since $\bar{M}(s) = \bar{f}(s)/s$ we have

$$M(t) \approx 0.007867 + 2.84078t - 0.945413t^2 + 0.193580t^3.$$

An alternative approach is to interpolate using Chebyshev polynomials. If we assume that s is real and greater than or equal to 1 then $1/s$ lies between 0 and 1 and, assuming that $\bar{f}(s)$ has an expansion in terms of $1/s$ we can reasonably expect $\bar{f}(s)$ to be representable in terms of a Chebyshev expansion

$$\bar{f}(s) = \frac{1}{2}a_0T_0^*(u) + \sum_{i=1}^{\infty} a_iT_i^*(u), \quad u = 1/s, \quad (10.15)$$

where the shifted Chebyshev polynomials satisfy

$$\begin{aligned} T_0^*(u) &= 1, & T_1^*(u) &= 2u - 1, \\ T_{i+1}^*(u) &= 2(2u - 1)T_i^*(u) - T_{i-1}^*(u). \end{aligned}$$

If we curtail the series (10.15) after N' terms and choose u_k to be the roots of the equation $T_{N'+1}^*(u) = 0$ we can get approximations for the coefficients in (10.15), namely,

$$a_i = \frac{2}{N' + 1} \sum_{k=1}^{N'+1} \bar{f}(s_k)T_i^*(u_k). \quad (10.16)$$

With $N' = 3$, for example, we obtain Table 10.2 and, applying (10.16), the coefficients are found to be

$$\begin{aligned} a_0 &= 2.06604 & a_1 &= 0.93784 \\ a_2 &= -0.07158 & a_3 &= 0.01548 \end{aligned}$$

so that

$$\begin{aligned} \bar{f}(s) &\approx 1.03302 + 0.93784 \left(\frac{2}{s} - 1 \right) - 0.07158 \left(\frac{8}{s^2} - \frac{8}{s} + 1 \right) \\ &\quad + 0.01548 \left(\frac{32}{s^3} - \frac{48}{s^2} + \frac{18}{s} - 1 \right). \end{aligned}$$

t	$M_5(t)$	$M_7(t)$	$M_{11}(t)$
1	2.09887	2.098898	2.09888998
5	7.21757	7.217428	7.21742866
10	12.63402	12.633765	12.63376729
15	17.80708	17.806697	17.80670042
20	22.89213	22.891567	22.89157171
25	27.93761	27.936815	27.93681966
30	32.96325	32.962193	32.96219778

Table 10.3: Estimates for $M(t)$ using the Gaver method.

Hence we obtain

$$\bar{M}(s) = \bar{f}(s)/s,$$

and, using the result $\mathcal{L}^{-1}\{1/s^{n+1}\} = t^n/n!$, we obtain

$$M(t) = 0.00812 + 2.72732t - 0.65784t^2 + 0.08256t^3.$$

We need not, of course, restrict ourselves to cubic polynomials.

3. The method of Gaver

This method has been described in Chapter 7. The function $\bar{M}(s)$ has to be evaluated at $s = r \ln 2/t$ for $r = n, n+1, \dots, 2n$. The numerical estimates obtained for $M(t)$, call them $M_n(t)$, are presented in Table 10.3 for a variety of n and t . Clearly, there is in this instance remarkable accuracy, even for small values of n , over the range of values of t which we have considered. We give a program for estimating $M(t)$ by the Gaver method at the URL www.cf.ac.uk/maths/cohen/programs/inverselaplace/transform/.

10.2 Application 2. Heat Conduction in a Rod

In order to study this problem we require a physical model. We make the assumption that heat is conceptually like a fluid and is free to flow from one position to another in a material. Its presence is measured by the temperature (as recorded on a thermometer) — the higher the temperature the more heat present. The flow of heat will be from places of higher temperature to places of lower temperature. The unit of heat (in cgs units) is called the calorie and is the amount of heat needed to raise the temperature of one gram of water one degree Centigrade.

There are two hypotheses about the nature of heat which have experimental support. The first, called the absorption hypothesis, states that the amount of increase, ΔQ , in the quantity of heat in a material is directly proportional to the mass m of the material and to the increase in temperature Δu , i.e.,

$$\Delta Q = cm\Delta u.$$

The constant of proportionality, c , is called the *specific heat* of the material and does not vary throughout the material. For water $c=1$ and for silver $c \approx 0.06$. The second hypothesis, called the conduction hypothesis, concerns a strip of length Δx of a rod of cross-section A whose sides are insulated and whose ends are held at two different temperatures. For convenience we shall imagine that we are dealing with the flow of heat along a uniform rod which has the same thermal properties throughout its length. Then in a small time Δt we find that ΔQ is proportional to A , $\Delta u/\Delta x$ and Δt , i.e.,

$$\Delta Q = -KA \frac{\Delta u}{\Delta x} \Delta t.$$

K , the constant of proportionality, is called the *thermal conductivity* of the material. For water $K \approx 0.0014$ and for silver $K \approx 1.0006$. It follows from the above, that in a section of material of mass m , the instantaneous rate of increase in the quantity of heat at some time t_0 is proportional to the instantaneous rise in temperature. That is

$$\left. \frac{\partial Q}{\partial t} \right|_{t_0} = cm \left. \frac{\partial u}{\partial t} \right|_{t_0}. \quad (10.17)$$

Likewise, the rate of flow across the surface $x = x_0$ at a given instant t_0 is proportional to the temperature gradient there. Thus

$$\left. \frac{\partial Q}{\partial t} \right|_{x_0} = -KA \left. \frac{\partial u}{\partial x} \right|_{x_0}. \quad (10.18)$$

Relating this to a segment of the rod between x_0 and $x_0 + \Delta x$ we see that the rate of absorption $\partial Q/\partial t$ at a given point x at time t_0 is proportional to $\partial u/\partial t$. The average value of $\partial u/\partial t$ over the segment occurs at some interior point $x_0 + \theta \Delta x$ giving, for the whole segment,

$$\left. \frac{\partial Q}{\partial t} \right|_{t=t_0} = c\rho \Delta x A \frac{\partial u}{\partial t}(x_0 + \theta \Delta x, t_0), \quad 0 < \theta < 1, \quad (10.19)$$

where ρ denotes the density of the material of the rod.

This rate of heat increase may be computed in another way as it is exactly the difference between the heat entering the segment at x_0 and leaving at $x_0 + \Delta x$ at time t_0 . That is, from (10.18),

$$\left. \frac{\partial Q}{\partial t} \right|_{t=t_0} = KA \left(\frac{\partial u}{\partial x}(x_0 + \Delta x, t_0) - \frac{\partial u}{\partial x}(x_0, t_0) \right). \quad (10.20)$$

The mean value theorem applied to the right-hand term of (10.20) shows that this term equals

$$KA \frac{\partial^2 u}{\partial x^2}(x_0 + \eta \Delta x, t_0) \Delta x, \quad 0 < \eta < 1.$$

Now, equating these results and letting Δx approach zero we obtain the equation

$$K \frac{\partial^2 u}{\partial x^2} = c\rho \frac{\partial u}{\partial t}, \quad (10.21)$$

where the derivatives are evaluated at (x_0, t_0) . Writing $\kappa = K/c\rho$ we obtain the one dimensional heat conduction equation

$$\kappa \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}. \quad (10.22)$$

κ was called the *thermometric conductivity* by Clerk Maxwell but Lord Kelvin referred to it as the *diffusivity*.

We now return to Example 2.4 where we established that

$$\bar{y}(x, s) = \frac{1}{s} e^{-x\sqrt{s}},$$

and contour integration yielded

$$y(x, t) = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{t}}\right) = \operatorname{erfc}(x/2\sqrt{t}).$$

Thus at time $t = 1$ and $x = 5$ we have $y \approx 0.0004069520$. We have evaluated $y(5, 1)$ by a number of methods and the results are given below:-

1. Crump's method

This was an application of NAG Library program C06LAF where, of course, the function subroutine has to evaluate $\mathcal{L}^{-1}\{\exp(-5\sqrt{s})/s\}$ at $t = 1$. With tfac=0.8, alphab=0.01 and relerr=0.001 a result of 0.000407 was obtained.

2. Weeks method

No results were obtainable for the Laplace transform given in this example using the NAG Library routines C06LBF and C06LCF. This failure derives from the fact that $y(x, t)$ does not have continuous derivatives of all orders.

3. Gaver's method

With $n = 7$ the estimate for $y(5, 1)$ was 0.0004062 while $n = 11$ yielded $y(5, 1) \approx 0.0004069537$.

10.3 Application 3. Laser Anemometry

McWhirter and Pike [154] consider the integral equation

$$g(\tau) = \int_0^\infty K(v\tau)p(v)dv, \quad 0 \leq \tau < \infty, \quad (10.23)$$

where the kernel K depends on the product of v and τ and has the property that

$$\int_0^\infty |K(x)|x^{-1/2}dx < \infty. \quad (10.24)$$

This class of equation includes the Laplace transform.

The eigenfunctions $\phi_\omega(v)$ and eigenvalues λ_ω satisfy

$$\int_0^\infty K(v\tau)\phi_\omega(v)dv = \lambda_\omega\phi_\omega(\tau). \quad (10.25)$$

McWhirter and Pike consider the function

$$\phi_s(v) = Av^{-s} + Bv^{s-1}, \quad (10.26)$$

where A, B and s are complex numbers, substituted in (10.23). This yields a function

$$g_s(\tau) = \int_0^\infty K(v\tau)(Av^{-s} + Bv^{s-1})dv,$$

which exists and is finite provided the integral converges. Making the substitution $z = v\tau$ we get

$$g_s(\tau) = \int_0^\infty K(z) \left[A \left(\frac{z}{\tau} \right)^{-s} + B \left(\frac{z}{\tau} \right)^{s-1} \right] \frac{dz}{\tau},$$

or

$$g_s(\tau) = A\tilde{K}(1-s)\tau^{s-1} + B\tilde{K}(s)\tau^{-s}, \quad (10.27)$$

where $\tilde{K}(s)$ is the Mellin transform of $K(x)$ defined by

$$\tilde{K}(s) = \int_0^\infty x^{s-1}K(x)dx.$$

If $\tilde{K}(s)$ exists for $\alpha < \Re s < \beta$ then it follows that $\tilde{K}(1-s)$ exists for $1-\beta < \Re s < 1-\alpha$ and thus equation (10.27) is properly defined for $\alpha \leq \frac{1}{2} \leq \beta$. Choosing

$$A = \sqrt{(\tilde{K}(s))}, \quad B = \pm\sqrt{(\tilde{K}(1-s))},$$

then

$$g_s(\tau) = \pm\sqrt{(\tilde{K}(s)\tilde{K}(1-s))}\phi_s(\tau),$$

and consequently the functions

$$\left. \begin{aligned} \phi_s^{(1)}(v) &= \sqrt{(\tilde{K}(s))}v^{-s} + \sqrt{(\tilde{K}(1-s))}v^{s-1} \\ \phi_s^{(2)}(v) &= \sqrt{(\tilde{K}(s))}v^{-s} - \sqrt{(\tilde{K}(1-s))}v^{s-1} \end{aligned} \right] \quad (10.28)$$

are eigenfunctions satisfying (10.25) with corresponding eigenvalues

$$\lambda_s^{(1)}, \lambda_s^{(2)} = \pm \sqrt{(\tilde{K}(s)\tilde{K}(1-s))}. \quad (10.29)$$

If we set $s = \frac{1}{2} + i\omega$ where ω is real and unbounded then introducing a convenient multiplicative factor yields a continuum of real eigenfunctions given by

$$\begin{aligned} \psi_\omega^{(1)}(v) &= \frac{\sqrt{(\tilde{K}(\frac{1}{2} + i\omega))}v^{-\frac{1}{2}-i\omega} + \sqrt{(\tilde{K}(\frac{1}{2} - i\omega))}v^{-\frac{1}{2}+i\omega}}{2\sqrt{(\pi|\tilde{K}(\frac{1}{2} + i\omega)|)}}, \\ &= \frac{\Re[\sqrt{(\tilde{K}(\frac{1}{2} + i\omega))}v^{-\frac{1}{2}-i\omega}]}{\sqrt{(\pi|\tilde{K}(\frac{1}{2} + i\omega)|)}}, \end{aligned} \quad (10.30)$$

and

$$\begin{aligned} \psi_\omega^{(2)}(v) &= \frac{\sqrt{(\tilde{K}(\frac{1}{2} + i\omega))}v^{-\frac{1}{2}-i\omega} - \sqrt{(\tilde{K}(\frac{1}{2} - i\omega))}v^{-\frac{1}{2}+i\omega}}{2i\sqrt{(\pi|\tilde{K}(\frac{1}{2} + i\omega)|)}}, \\ &= \frac{\Im[\sqrt{(\tilde{K}(\frac{1}{2} + i\omega))}v^{-\frac{1}{2}-i\omega}]}{\sqrt{(\pi|\tilde{K}(\frac{1}{2} + i\omega)|)}}, \end{aligned} \quad (10.31)$$

with real eigenvalues

$$\lambda_\omega^{(1)}, \lambda_\omega^{(2)} = \pm |\tilde{K}(\frac{1}{2} + i\omega)|. \quad (10.32)$$

These functions are well defined provided that the transform $\tilde{K}(\frac{1}{2} + i\omega)$ exists and a sufficient condition for this is (10.24). Moreover, because of the symmetry relationships

$$\left. \begin{aligned} \psi_\omega^{(1)}(v) &= \psi_{-\omega}^{(1)}(v) \\ \psi_\omega^{(2)}(v) &= -\psi_{-\omega}^{(2)}(v) \end{aligned} \right] \quad (10.33)$$

we need only consider $\omega \geq 0$.

McWhirter and Pike proceed to show that the eigenfunctions are not normalisable but are mutually orthogonal in the sense that

$$\begin{aligned} \int_0^\infty \psi_\omega^{(1)}(v)\psi_{\omega'}^{(1)}(v)dv &= \begin{cases} \delta(\omega - \omega') & \text{if } \omega \neq 0 \\ 2\delta(\omega) & \text{if } \omega = 0 \end{cases} \\ \int_0^\infty \psi_\omega^{(2)}(v)\psi_{\omega'}^{(2)}(v)dv &= \begin{cases} \delta(\omega - \omega') & \text{if } \omega \neq 0 \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

and also

$$\int_0^\infty \psi_\omega^{(1)}(v)\psi_{\omega'}^{(2)}(v)dv = 0.$$

They also give expressions for $\psi_\omega^{(1)}(v)$ and $\psi_\omega^{(2)}(v)$. If $p(v)$ is a piecewise continuous function for which $\int_0^\infty |p(v)|v^{-1/2}dv$ exists then we can express $p(v)$ in terms of the eigenfunctions, i.e.,

$$p(v) = \int_0^\infty a_\omega^{(1)}\psi_\omega^{(1)}(v)d\omega + \int_0^\infty a_\omega^{(2)}\psi_\omega^{(2)}(v)d\omega, \quad (10.34)$$

where

$$\left. \begin{aligned} a_{\omega}^{(1)} &= \int_0^{\infty} p(v) \psi_{\omega}^{(1)}(v) dv \\ a_{\omega}^{(2)} &= \int_0^{\infty} p(v) \psi_{\omega}^{(2)}(v) dv \end{aligned} \right] \quad (10.35)$$

Substitution of (10.34) in (10.23) gives

$$g(\tau) = \int_0^{\infty} a_{\omega}^{(1)} \lambda_{\omega}^{(1)} \psi_{\omega}^{(1)}(\tau) d\omega + \int_0^{\infty} a_{\omega}^{(2)} \lambda_{\omega}^{(2)} \psi_{\omega}^{(2)}(\tau) d\omega, \quad (10.36)$$

and from the orthogonality relationships it follows that

$$a_{\omega}^{(i)} = \frac{1}{\lambda_{\omega}^{(i)}} \int_0^{\infty} g(\tau) \psi_{\omega}^{(i)}(\tau) d\tau, \quad i = 1, 2, \quad (10.37)$$

and hence

$$\begin{aligned} p(v) &= \int_0^{\infty} d\omega \psi_{\omega}^{(1)}(v) \frac{1}{\lambda_{\omega}^{(1)}} \int_0^{\infty} d\tau \psi_{\omega}^{(1)}(\tau) g(\tau) \\ &\quad + \int_0^{\infty} d\omega \psi_{\omega}^{(2)}(v) \frac{1}{\lambda_{\omega}^{(2)}} \int_0^{\infty} d\tau \psi_{\omega}^{(2)}(\tau) g(\tau). \end{aligned} \quad (10.38)$$

This solution parallels that of (8.8) the discrete summation being replaced by an integral since (10.23) has an infinite continuum of eigenvalues. As mentioned in Chapter 8 it is impossible to gain any information about those components of $p(v)$ for which $\omega > \omega_{\max}$ and the solution must therefore be written as

$$\begin{aligned} p(v) &= \int_0^{\omega_{\max}} d\omega \psi_{\omega}^{(1)}(v) \frac{1}{\lambda_{\omega}^{(1)}} \int_0^{\infty} d\tau \psi_{\omega}^{(1)}(\tau) g(\tau) \\ &\quad + \int_0^{\omega_{\max}} d\omega \psi_{\omega}^{(2)}(v) \frac{1}{\lambda_{\omega}^{(2)}} \int_0^{\infty} d\tau \psi_{\omega}^{(2)}(\tau) g(\tau) \\ &\quad + \int_{\omega_{\max}}^{\infty} d\omega \alpha_{\omega}^{(1)} \psi_{\omega}^{(1)}(v) + \int_{\omega_{\max}}^{\infty} d\omega \alpha_{\omega}^{(2)} \psi_{\omega}^{(2)}(v), \end{aligned} \quad (10.39)$$

where ω_{\max} depends on errors during calculation or in measuring $g(\tau)$ and the coefficients $\alpha_{\omega}^{(i)}$, $i = 1, 2$ must be determined by some *a priori* knowledge of the result and cannot be evaluated independently.

McWhirter and Pike note that the solution of equation (10.23) can be obtained more directly by taking the Mellin transform of both sides. As the integral is a Mellin convolution this gives

$$\tilde{g}(s) = \tilde{K}(s) \tilde{p}(1-s),$$

and thus

$$\tilde{p}(s) = \tilde{g}(1-s) / \tilde{K}(1-s).$$

The transform of $p(v)$ is analytic for $\Re(s) = \frac{1}{2}$ and from the inversion formula for the inverse Mellin transforms it follows that

$$p(v) = \frac{1}{2\pi i} \int_{\frac{1}{2}-i\infty}^{\frac{1}{2}+i\infty} v^{-s} \frac{\tilde{g}(1-s)}{\tilde{K}(1-s)} ds. \quad (10.40)$$

From this result we can recover the equation (10.38) by making the substitution $s = \frac{1}{2} + i\omega$, expressing (10.40) as a double integral and then formulating in terms of the eigenfunctions.

McWhirter and Pike consider the example of the equation

$$g(\tau) = \int_0^\infty e^{-\alpha v \tau} \cos(\beta v \tau) p(v) dv,$$

and observe that, in the limit $\alpha \rightarrow 0$, this takes the form of a Fourier cosine transform while in the limit $\beta \rightarrow 0$ it becomes a Laplace transform. From (10.29) they are able to determine the rate at which the eigenvalues decay to zero. In the case $\beta \rightarrow 0$ they determine that the eigenvalue ‘spectrum’, more specifically, $|\lambda_\omega^{(i)}|^2$, decays proportionally to $e^{-\pi\omega}$ for large ω . When $\alpha = 0$ they show

$$|\lambda_\omega^{(i)}|^2 = \frac{\pi}{2\beta}$$

which never decays to zero. This analysis showed that the Fourier transform has a much greater information capacity than the Laplace transform.

To illustrate the application of the above theory McWhirter and Pike consider the numerical solution of the equation

$$g(\tau) = \frac{(1 + \tau)^2 - \beta^2 \tau^2}{[(1 + \tau)^2 + \beta^2 \tau^2]^2} = \int_0^\infty e^{-v\tau} \cos(\beta v \tau) p(v) dv. \quad (10.41)$$

whose exact solution is known to be

$$p(v) = v e^{-v},$$

but no knowledge of this was assumed during their calculations. These were based on the use of equation (10.39) and the undetermined parameters α_ω being set to zero as in the truncation method of regularization. Crucial to the whole exercise was the choice of ω_{\max} and they examined the results obtained by varying ω_{\max} under varying conditions of noise (in the data) and information capacity (i.e. β). Also, to evaluate the eigenfunction projection integrals (10.37) it is convenient to replace the lower limit by L_1 (since $\psi_\omega^{(i)}(\tau)$ is not defined at $\tau = 0$) and the upper limit by L_2 but at the same time ensuring that the truncation error which results does not significantly affect the computation. By choosing

$$L_1 = 10^{-15}, \quad L_2 = 10^5,$$

we have

$$\left| \int_0^{L_1} g(\tau) \psi_\omega^{(i)}(\tau) d\tau \right| \leq \frac{1}{\sqrt{\pi}} \int_0^{L_1} |g(\tau)| \tau^{-1/2} d\tau \sim L_1^{1/2}, \quad i = 1, 2$$

and

$$\left| \int_{L_2}^\infty g(\tau) \psi_\omega^{(i)}(\tau) d\tau \right| \leq \frac{1}{\sqrt{\pi}} \int_{L_2}^\infty |g(\tau)| \tau^{-1/2} d\tau \sim L_2^{-3/2}, \quad i = 1, 2$$

and the truncation errors are thus of order $10^{-7.5}$. As the quadrature routine used by McWhirter and Pike evaluated the integrals correctly to an accuracy of 10^{-5} the truncation error was of no consequence.

If

$$\Delta\omega = 2\pi/[\ln(L_2) - \ln(L_1)], \quad (10.42)$$

it can be shown that the discrete subset of eigenfunctions

$$\psi_{n\Delta\omega}^{(i)}, \quad i = 1, 2; \quad n = 0, 1, 2, \dots$$

form a complete orthogonal set on the interval $[L_1, L_2]$ and may be normalised by the factor $\Delta\omega^{1/2}$. As a result the calculations reduced to the evaluation of the discrete finite sums

$$p_N(v) = \sum_{n=0}^N \frac{c_n^{(1)}}{\lambda_{n\Delta\omega}^{(1)}} \psi_{n\Delta\omega}^{(1)}(v) + \sum_{n=1}^N \frac{c_n^{(2)}}{\lambda_{n\Delta\omega}^{(2)}} \psi_{n\Delta\omega}^{(2)}(v), \quad (10.43)$$

where

$$c_n^{(i)} = \begin{cases} \Delta\omega \int_{L_1}^{L_2} g(\tau) \psi_{n\Delta\omega}^{(i)}(\tau) d\tau, & n \neq 0 \\ \frac{1}{2} \Delta\omega \int_{L_1}^{L_2} g(\tau) \psi_0(\tau) d\tau, & n = 0 \end{cases} \quad i = 1, 2 \quad (10.44)$$

with

$$\Delta\omega \simeq 0.136 \quad \text{and} \quad N\Delta\omega = \omega_{\max}. \quad (10.45)$$

The uniform discretisation was particularly convenient in this example as the value of ω_{\max} in which we are interested is then directly proportional to N , the number of terms retained in the series. McWhirter and Pike evaluated the eigenfunction projections (10.44) by first making the substitution $\tau = e^x$ in order to obtain better conditioning of the integrals which were then evaluated using a four-point Gauss quadrature formula. They remark that it is not possible to evaluate $p_N(v)$ when $v = 0$ because $\psi_{n\Delta\omega}^{(i)}(v)$ is singular.

Of particular interest to us is the case $\beta = 0$ in equation (10.41) which, as stated earlier, corresponds to finding an inverse Laplace transform. Two cases were considered and the results obtained by McWhirter and Pike are shown graphically in Figures 10.1 and 10.2.

Case 1. Calculation of the eigenfunction components of $g(\tau)$ not subject to any noise apart from the small error ($\sim 10^{-5}$) incurred during the integration process.

Case 2. Identical with Case 1 except for the calculated eigenfunction components being subjected to the addition of Gaussian random errors with standard deviation 10^{-3} .

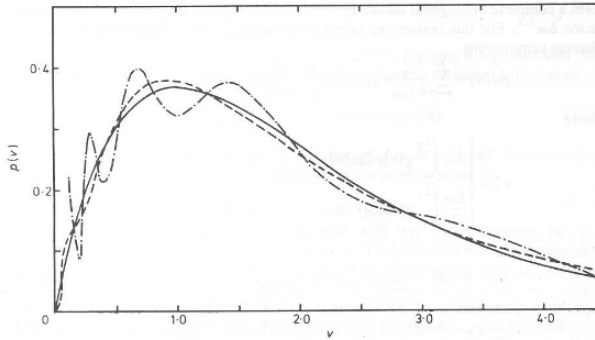


Figure 10.1: $p_N(v)$ as a function of v . $\beta = 0$ and noise $\sim 10^{-5}$: broken curve, $N = 20$; chain curve, $N = 60$; full curve, actual solution $p(v) = ve^{-v}$ (and $N = 40$) (Reproduced from [154] with permission)

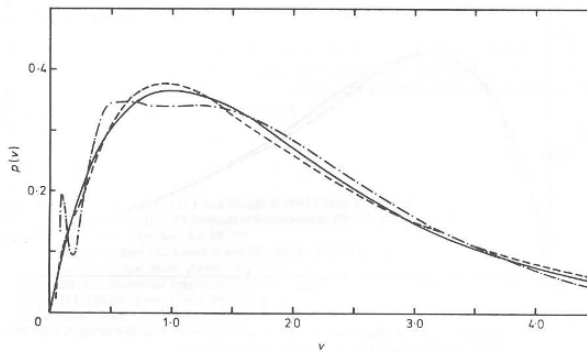


Figure 10.2: $p_N(v)$ as a function of v . $\beta = 0$ and noise $\sim 10^{-3}$: broken curve, $N = 20$; chain curve, $N = 30$; full curve, actual solution $p(v) = ve^{-v}$ (Reproduced from [154] with permission)

In a subsequent paper McWhirter [153] looked at the problem of solving the integral equation

$$g(\tau) = A \int_0^\infty e^{-v^2 \tau^2 / r^2} \left[1 + f \cos \left(\frac{2\pi v \tau}{s_0} \right) \right] p(v) dv + c, \quad (10.46)$$

which is, apart from the term c which denotes experimental background level, an equation of the form (10.23). The exponential term arises from the gaussian profile (assumed to have width r) of the laser beams and the cosine term is associated with the virtual fringe pattern whose visibility factor is f and fringe spacing is s_0 . A is a simple scaling factor and whereas previously we virtually

had an explicit formulation for $g(\tau)$, the correlation function is now defined by the sample

$$g(\tau_i) = g(iT), \quad i = 1, 2, \dots, N \quad (10.47)$$

where T is the correlation time and N is the number of channels used. McWhirter uses a simple histogram model to deal with this situation and mentions that in some situations it would be appropriate to model the data using cubic B-spline functions.

10.4 Application 4. Miscellaneous Quadratures

The application of Laplace transforms to evaluate integrals involving a parameter is something which is not new. However, most of the examples cited involve transforms which are known from tables. Abramowitz [4] gives the example of the function $f(x)$ defined by the integral

$$f(x) = \int_0^\infty \frac{e^{-u^2} du}{x+u}. \quad (10.48)$$

If the substitution $u = xv$ is made and x^2 is replaced by t we obtain

$$g(t) = \int_0^\infty \frac{e^{-tv^2}}{1+v} dv.$$

The Laplace transform of $g(t)$ with respect to t is

$$\int_0^\infty \frac{dv}{(1+v)(s+v^2)} = \frac{\pi}{2\sqrt{s(s+1)}} + \frac{\ln s}{2(s+1)}.$$

Abramowitz writes that, by consulting the tables in Doetsch [68], we have

$$\mathcal{L}^{-1} \left\{ \frac{1}{\sqrt{s(s+1)}} \right\} = \frac{2e^{-t}}{\sqrt{\pi}} \int_0^{t^{1/2}} e^{u^2} du, \quad \mathcal{L}^{-1} \left\{ \frac{\ln s}{(s+1)} \right\} = -e^{-t} \text{Ei}(t),$$

where $\text{Ei}(t)$ is the exponential integral. It follows that

$$f(x) = \sqrt{\pi} e^{-x^2} \int_0^x e^{u^2} du - \frac{1}{2} e^{-x^2} \text{Ei}(x^2). \quad (10.49)$$

This technique is particularly useful when the integrand contains an oscillatory term such as $\cos tx$, $\sin tx$ or $J_n(tx)$. For example, if

$$I_1(t) = \int_0^\infty \frac{\sin tx}{x+1} dx, \quad (10.50)$$

then

$$\mathcal{L}\{I_1(t)\} = \int_0^\infty e^{-st} \left(\int_0^\infty \frac{\sin tx}{x+1} dx \right) ds. \quad (10.51)$$

Interchange of the variables is permissible here if $\Re s > 0$ and consequently

$$\begin{aligned} \bar{I}_1(s) &= \int_0^\infty \frac{1}{x+1} \left(\int_0^\infty e^{-st} \sin tx dt \right) dx, \\ &= \int_0^\infty \frac{x}{(s^2+x^2)(x+1)} dx. \end{aligned} \quad (10.52)$$

The integrand in (10.52) can be put in the form

$$\frac{1}{s^2+1} \left[\left(\frac{x}{s^2+x^2} - \frac{1}{x+1} \right) + \frac{s^2}{s^2+x^2} \right],$$

and integration yields

$$\bar{I}_1(s) = \frac{\ln s}{s^2 + 1} + \frac{\frac{1}{2}\pi s}{s^2 + 1}. \quad (10.53)$$

By consulting the tables in Roberts and Kaufman [197] we find that

$$I_1(t) = (\tfrac{1}{2}\pi + \text{Si}(t)) \cos t - \text{Ci}(t) \sin t, \quad (10.54)$$

where $\text{Ci}(t)$ and $\text{Si}(t)$ are respectively the Cosine and Sine integrals

$$\text{Ci}(t) = C + \ln t + \int_0^t \frac{\cos u - 1}{u} du, \quad \text{Si}(t) = \int_0^t \frac{\sin u}{u} du,$$

— see Abramowitz and Stegun [5]. Even if one didn't know the solution in terms of Sine and Cosine integrals one could use the techniques given in this book to determine $I_1(t)$ for a range of t .

Another example which was studied by the author [41] concerns the computation of the creep function $\phi(t)$ which satisfies the integral equation

$$B(x) = \int_0^\infty \phi(t) \sin xtdt, \quad (10.55)$$

where $B(x)$ is the dielectric loss factor represented by

$$B(x) = \frac{Ax^\alpha}{1 + x^{2\alpha}}, \quad 0 < \alpha \leq 1.$$

Application of the Fourier sine inversion theorem yields

$$\phi(t) = \frac{2A}{\pi} \int_0^\infty \frac{x^\alpha}{1 + x^{2\alpha}} \sin tx dx, \quad t > 0.$$

Thus apart from a constant factor, the function

$$I_2(\alpha, t) = \int_0^\infty \frac{x^\alpha}{1 + x^{2\alpha}} \sin tx dx, \quad t > 0, \quad (10.56)$$

determines the creep function $\phi(t)$. We can get an explicit formula for $\alpha = 1$ by straightforward contour integration, namely

$$I_2(1, t) = \frac{\pi}{2} e^{-t}.$$

We can also use Laplace transforms to determine the value of $I_2(\frac{1}{2}, t)$. Proceeding as above we find

$$\bar{I}_2(\tfrac{1}{2}, s) = \mathcal{L}\{I_2(\tfrac{1}{2}, t)\} = \int_0^\infty \frac{x^{3/2} dx}{(1+x)(s^2+x^2)}.$$

By the application of the result (Whittaker and Watson [250] p.117 et seq.)

$$\int_0^\infty x^{a-1} Q(x) dx = \pi \operatorname{cosec} a\pi \sum \text{residues of } Q(z),$$

where it is assumed that $x^a Q(x) \rightarrow 0$ as $x \rightarrow 0$ and $x \rightarrow \infty$ and the function $(-a)^{a-1} Q(z)$ is integrated around a keyhole contour, we obtain

$$\begin{aligned} \bar{I}_2(\tfrac{1}{2}, s) &= \frac{\pi}{s^2 + 1} + \frac{\pi s^{1/2}(s-1)}{\sqrt{2}(s^2 + 1)}, \\ &= \frac{\pi}{s^2 + 1} + \frac{\pi}{\sqrt{2}s} - \frac{\pi}{\sqrt{2}s} \left(\frac{s}{s^2 + 1} + \frac{1}{s^2 + 1} \right). \end{aligned} \quad (10.57)$$

The last term on the right hand side is, apart from the constant factor, the product of the transforms of $1/\sqrt{\pi t}$ and $(\cos t + \sin t)$ and thus the convolution theorem enables us to establish a closed form result for $I_2(\frac{1}{2}, t)$, namely

$$I_2(\tfrac{1}{2}, t) = \pi \sin t + \sqrt{(\pi/2t) - \sqrt{2\pi}} \{(\cos t + \sin t)C(\sqrt{t}) + (\sin t - \cos t)S(\sqrt{t})\}, \quad (10.58)$$

where $C(t)$ and $S(t)$ are the Fresnel integrals

$$C(t) = \int_0^t \cos(u^2) du, \quad S(t) = \int_0^t \sin(u^2) du.$$

For other values of α we obtain the integral

$$\bar{I}_2(\alpha, t) = \int_0^\infty \frac{x^{1+\alpha} dx}{(1+x^{2\alpha})(s^2+x^2)},$$

which, apart from some exceptional values of α , such as $\alpha = \frac{1}{4}$, is quite formidable to compute. In this instance it is preferable to deal with the original integral $I(\alpha, t)$ and apply the method of §11.3 to evaluate the integral — care, however, must be taken in evaluating the first term of the sequence because of the singularity at the origin.

The earlier examples were all infinite integrals but we can treat a wider range of integrals. Talbot [226] cites the examples of Burnett and Soroka [28] which arose in modelling a problem in Acoustics. If we just consider the cosine integral (the sine integral can be treated similarly)

$$C(t, R) = \int_c^d \sqrt{1 - R/x^2} \cos tx dx, \quad c = \sqrt{R}, \quad d = \sqrt{R + 1/R} \quad (10.59)$$

then

$$\bar{C}(s, R) = \int_c^d \left(\int_0^\infty e^{-st} \cos tx dt \right) \sqrt{1 - R/x^2} dx,$$

yielding

$$\bar{C}(s, R) = \int_c^d \frac{s}{s^2 + x^2} \sqrt{1 - R/x^2} dx.$$

By making the substitution $x = \sqrt{R} \operatorname{cosec} \theta$ this integral becomes

$$\sqrt{R} \int_{\frac{\pi}{2}-\varphi}^{\frac{\pi}{2}} \frac{s \cot^2 \theta d\theta}{s^2 + R \operatorname{cosec}^2 \theta}, \quad \text{where } \sec \phi = \sqrt{(1 + 1/R^2)}.$$

A little manipulation produces the result

$$\bar{C}(s, R) = \sqrt{R}(s + R/s) \int_{\frac{\pi}{2}-\varphi}^{\frac{\pi}{2}} \frac{d\theta}{s^2 \sin^2 \theta + R} - \frac{\varphi \sqrt{R}}{s}.$$

From Gradshteyn and Ryzhik [102] we have the result

$$\int \frac{dx}{a + b \sin^2 x} = \frac{1}{\sqrt{a(a+b)}} \arctan \left(\sqrt{\frac{a+b}{a}} \tan x \right), \quad a, b > 0$$

and hence we can obtain an explicit expression for $\bar{C}(s, R)$, namely,

$$\bar{C}(s, R) = \frac{\pi \sqrt{(R + s^2)}}{2s} - \frac{\sqrt{(R + s^2)}}{s} \arctan \left(\sqrt{\frac{R + s^2}{R^3}} \right) - \frac{\varphi \sqrt{R}}{s}. \quad (10.60)$$

$C(t, R)$ can then be determined for given t by numerical evaluation of the inverse transform.

10.5 Application 5. Asian Options

An **option** is the right (but not the obligation) to buy or sell a risky asset, such as a stock or a parcel of shares, at a pre-specified price within a specified period (Seydel [207]). Options have a limited life time. The *maturity date* T fixes the time at which the rights of the holder expire and for $t > T$ the option is worthless. There are two basic types of option. The **call** option gives the holder the right to buy the asset, whose price at time t will be denoted by S or S_t , for an agreed price K (K is the unit price of the asset) by the date T . The **put** option gives the holder the right to sell the asset at a price K (which is different from the call option price) by the date T . The price K is called the **strike** or **exercise price**. There are two aspects of options and they relate to either the holder or the bank/stockbroker which underwrites the option. The latter have an obligation to buy/sell the asset at the strike price K if the holder decides to exercise the option but their risk situation is different from that of the holder as they receive a premium when they underwrite the option and this compensates for any future potential liabilities. This application investigates options from the standpoint of the holder.

Options have been given designations relating to continents. **European** options can only be exercised at the expiry date T . **American** options can be exercised at any time until the expiry date. **Asian** options give the holder the right to buy an asset for its average price over some prescribed period. With all these types of options we want to be able to estimate the **pay-off** function $V(S, t)$ which in the case of a European call option only has validity when $t = T$ and is defined by

$$V(S, T) = \begin{cases} 0, & S \leq K \quad (\text{option is worthless}) \\ S - K, & S > K \quad (\text{option exercised}) \end{cases}$$

or

$$V(S, T) = \max(S - K, 0) = (S - K)^+. \quad (10.61)$$

Similarly for a European put option

$$V(S, T) = (K - S)^+. \quad (10.61')$$

The fact that the pay-off function is positive when the option is exercised does not necessarily imply that the holder of the option makes a profit. This is because the initial costs paid when buying the option have to be subtracted. One also has to take into account that the money could have been invested over the option period at some interest rate r in order to work out whether the taking out of the option was profitable to the holder.

Likewise the pay-off function for an American call option is $(S_t - K)^+$ and for an American put $(K - S_t)^+$ where t denotes any time $\leq T$. With Asian options we need to determine the average value of S_t . This can be done by observing S_t at discrete time intervals, say $t_k = k(T/n)$, $k = 1, \dots, n$ and then determining the arithmetic mean

$$\frac{1}{n} \sum_{k=1}^n S_{t_k}.$$

If the observations are continuously sampled in the period $0 \leq t \leq T$, the arithmetic mean corresponds to

$$\hat{S} = \frac{1}{T} \int_0^T S_t dt. \quad (10.62)$$

An alternative approach, which is sometimes used, is to consider the geometric average which is defined by

$$\left(\prod_{k=1}^n S_{t_k} \right)^{1/n} = \exp \left(\frac{1}{n} \ln \prod_{k=1}^n S_{t_k} \right) = \exp \left(\frac{1}{n} \sum_{k=1}^n \ln S_{t_k} \right).$$

For continuously sampled observations this can be expressed in the form

$$\hat{S}_g = \exp \left(\frac{1}{T} \int_0^T \ln S_t dt \right). \quad (10.63)$$

The averages (10.62), (10.63) have been formulated for the time period $0 \leq t \leq T$ and thus corresponds to a European option. To allow for early exercise of the option as with American options we have to modify (10.62) and (10.63) appropriately. Thus, for example, (10.62) now becomes

$$\hat{S} = \frac{1}{t} \int_0^t S_u du.$$

We can define the pay-off function for Asian options as

$$(\hat{S} - K)^+ \quad \text{average price call}$$

$$(K - \hat{S})^+ \quad \text{average price put}$$

The above averages can be expressed in integral form by

$$A_t = \int_0^t f(S_u, u) du, \quad (10.64)$$

where the function $f(S, u)$ corresponds to the type of average chosen. In particular, if (10.62) holds then, apart from a scaling factor, $f(S, u) = S$. For Asian options the price V is a function of S , A and t and it is shown in Seydel [207] that V satisfies the partial differential equation

$$\frac{\partial V}{\partial t} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} + f(S, t) \frac{\partial V}{\partial A} - rV = 0. \quad (10.65)$$

The quantities r and σ in the above equation denote respectively interest rate and volatility. The above equation has been solved approximately by applying the classical methods of Numerical Analysis for the solution of partial differential equations — see, for example, Rogers and Shi [198].

Geman and Yor [94] established that the problem of valuing Asian options could

be tackled by Laplace transform evaluation. Calculations have been performed by Fu et al [90], Carr and Schröder [30] and Craddock et al [52] and others using a variety of numerical methods for the inversion of Laplace transforms but, at this point in time, results have not been very satisfactory. Essentially, we are trying to determine the price $C(t)$ of the Asian option which is defined by

$$C(t) = \frac{4e^{-r(T-t)}S(t)}{\sigma^2(T-t_0)}C^{(\nu)}(h, q), \quad (10.66)$$

where r is the constant interest rate,

$$\nu = \frac{2r}{\sigma^2} - 1, \quad h = \frac{1}{4}\sigma^2(T-t), \quad q = \frac{\sigma^2}{4S(t)} \left(K(T-t_0) - \int_{t_0}^t S(u)du \right), \quad (10.67)$$

and the Laplace transform of $C^{(\nu)}(h, q)$ with respect to the h variable is

$$\begin{aligned} \bar{C}^{(\nu)}(s, q) &= \int_0^\infty e^{-sh} C^{(\nu)}(h, q) dh, \\ &= \frac{\int_0^{1/2q} e^{-x} x^{\frac{1}{2}(\mu-\nu)-2} (1-2qx)^{\frac{1}{2}(\mu+\nu)+1} dx}{s(s-2-2\nu)\Gamma(\frac{1}{2}(\mu-\nu)-1)}, \end{aligned} \quad (10.68)$$

where Γ denotes the gamma function and $\mu = \sqrt{2s + \nu^2}$. Since the integral in (10.68) requires $\frac{1}{2}(\mu-\nu)-2 > -1$ it is necessary to apply the shift theorem in order to weaken the singularity at the origin. To this end we redefine μ to be $\mu' = \sqrt{2(s+\alpha) + \nu^2}$ where $\alpha > 2 + 2\nu$. If we make the substitution $u = 2qx$ in the integral

$$\int_0^{1/2q} e^{-x} x^{\frac{1}{2}(\mu'-\nu)-2} (1-2qx)^{\frac{1}{2}(\mu'+\nu)+1} dx,$$

we obtain

$$\frac{1}{(2q)^{\frac{1}{2}(\mu'-\nu)-1}} \int_0^1 e^{-u/2q} u^{\frac{1}{2}(\mu'-\nu)-2} (1-u)^{\frac{1}{2}(\mu'+\nu)+1} du.$$

Application of the result (Abramowitz and Stegun [5])

$$\frac{\Gamma(b-a)\Gamma(a)}{\Gamma(b)} M(a, b, z) = \int_0^1 e^{zu} u^{a-1} (1-u)^{b-a-1} du, \quad \Re(b) > \Re(a) > 0, \quad (10.69)$$

where $M(a, b, z)$ is the Kummer confluent hypergeometric function, gives the Laplace transform to be inverted in the form

$$\bar{C}^{(\nu)}(s+\alpha) = \frac{(1/2q)^{\frac{1}{2}(\mu'-\nu)-1} \Gamma[\frac{1}{2}(\mu'+\nu) + 2] M(\frac{1}{2}(\mu'-\nu) - 1, \mu' + 1, -1/(2q))}{(s+\alpha)(s+\alpha-2-2\nu)\Gamma(\mu'+1)}. \quad (10.70)$$

Now

$$M(a, b, z) = 1 + \frac{az}{b} + \frac{(a)_2 z^2}{(b)_2 2!} + \cdots + \frac{(a)_n z^n}{(b)_n n!} + \cdots,$$

Case	r	σ	$T - t_0$	K	$S(t_0)$	q
1	0.05	0.5	1	2	1.9	0.06579
2	0.05	0.5	1	2	2	0.0625
3	0.05	0.5	1	2	2.1	0.05952
4	0.02	0.1	1	2	2	0.0025
5	0.18	0.3	1	2	2	0.0225
6	0.0125	0.25	2	2	2	0.03125
7	0.05	0.5	2	2	2	0.125

Table 10.4: Values for Asian option parameters

where $(a)_n$ is the Pochhammer symbol, i.e.,

$$(a)_n = a(a+1) \cdots (a+n-1) = \Gamma(n+a)/\Gamma(a), \quad (a)_0 = 1.$$

Substituting the series for M in (10.70) yields

$$\bar{C}^{(\nu)}(s+\alpha) = \frac{(1/2q)^{\frac{1}{2}(\mu'-\nu)-1} \Gamma[\frac{1}{2}(\mu'+\nu)+2] \Gamma[\frac{1}{2}(\mu'-\nu)-1]}{(s+\alpha)(s+\alpha-2-2\nu)\Gamma(\mu'+1)^2} \sum_{k=0}^{\infty} \rho_k, \quad (10.71)$$

where

$$\rho_0 = 1, \quad \rho_{k+1} = \frac{-1}{2q(k+1)} \left(\frac{\frac{1}{2}(\mu'-\nu) + k - 1}{\mu' + k + 1} \right) \rho_k.$$

Craddock et al [52] point out the difficulty of computing the series $\sum_{k=0}^{\infty} \rho_k$ when q is small as, with direct summation, 150 terms are needed to attain accuracy of the order of 10^{-4} when $q = 0.015$. With q less than 0.01 thousands of terms are needed to produce even one decimal place accuracy. As we have mentioned previously it is necessary to be able to evaluate the Laplace transform function accurately in order to overcome the ill-conditioning inherent in the numerical methods of inversion. In this instance we note that the criteria given by Sidi [216] for the satisfactory performance of the $W^{(m)}$ -algorithm are satisfied and we can thus sum the series accurately with far fewer terms needed. In the course of time this author hopes to be able to present his results for a selection of parameters which have been published by other researchers. Some typical values are given in Table 10.4. In Table 10.5 we give the Asian option prices obtained by Abate and Whitt [3], Eydeland and Geman [83], Turnbull and Wakeman [235] and Craddock et al [52] which will be denoted respectively by AW, EG, TW and CHP. Abate and Whitt used a trapezium rule approximation to the Bromwich integral, Eydeland and Geman employed a fast Fourier transform method, Turnbull and Wakeman gave an approximation formula and Craddock et al used an alternative quadrature routine from the Mathematica Library.

Case	AW	EG	TW	CHP
1	0.194	0.195	0.195	0.194
2	0.248	—	0.251	0.247
3	0.308	0.308	0.311	0.307
4	0.055	0.058	0.056	—
5	0.222	0.227	0.220	0.243
6	0.172	0.172	0.173	0.175
7	0.340	0.351	0.359	0.355

Table 10.5: Asian option prices

Chapter 11

Appendix

11.1 Table of Laplace Transforms

Function	Laplace Transform
$f(t)$	$\bar{f}(s)$
$af(t) + bg(t)$	$a\bar{f}(s) + b\bar{g}(s)$
$f(at)$	$\frac{1}{a}\bar{f}\left(\frac{s}{a}\right), \quad a > 0$
$e^{-\alpha t}f(t)$	$\bar{f}(s + \alpha)$
$f'(t)$	$s\bar{f}(s) - f(0+)$
$tf(t)$	$-\bar{f}'(s)$
$\int_0^t f(u)du$	$\frac{1}{s}\bar{f}(s)$
$\frac{f(t)}{t}$	$\int_s^\infty \bar{f}(x)dx$
$(f_1 * f_2)(t) = \int_0^t f_1(t-u)f_2(u)du$	$\bar{f}_1(s)\bar{f}_2(s)$
1	$\frac{1}{s}$
$H(t)$	$\frac{1}{s}$
t^n	$\frac{n!}{s^{n+1}}, \quad n = 0, 1, \dots$
t^ν	$\frac{\Gamma(\nu+1)}{s^{\nu+1}}, \quad \Re \nu > -1$

Function	Laplace Transform
$e^{-\alpha t}$	$\frac{1}{s + \alpha}$
$e^{-\alpha t} t^n$	$\frac{n!}{(s + \alpha)^{n+1}}, \quad n = 0, 1, \dots$
$H(t - a)$	$\frac{e^{-as}}{s}, \quad a > 0$
$H(t - a)f(t - a)$	$e^{-as}\bar{f}(s), \quad a > 0$
$\delta(t)$	1
$\cos at$	$\frac{s}{s^2 + a^2}$
$\sin at$	$\frac{a}{s^2 + a^2}$
$t \sin at$	$\frac{2as}{(s^2 + a^2)^2}$
$\sin at - at \cos at$	$\frac{2a^3}{(s^2 + a^2)^2}$
$\sinh at$	$\frac{a}{s^2 - a^2}$
$\cosh at$	$\frac{s}{s^2 - a^2}$
$e^{-\alpha t} \sin at$	$\frac{a}{(s + \alpha)^2 + a^2}$
$e^{-\alpha t} \cos at$	$\frac{s + \alpha}{(s + \alpha)^2 + a^2}$

Function	Laplace Transform
$L_n(t)$	$\frac{(s-1)^n}{s^{n+1}}$
$\frac{\sin t}{t}$	$\tan^{-1}\left(\frac{1}{s}\right)$
$J_0(t)$	$\frac{1}{\sqrt{s^2+1}}$
$J_n(t)$	$\frac{(\sqrt{s^2+1}-s)^n}{\sqrt{s^2+1}}$
$J_n(t)/t$	$(\sqrt{s^2+1}-s)^n/n \quad (n > 0)$
$t^{n-\frac{1}{2}}J_{n-\frac{1}{2}}(t)$	$\frac{2^{n-\frac{1}{2}}(n-1)!}{\sqrt{\pi}(s^2+1)^n} \quad (n > 0)$
$J_0(2\sqrt{at})$	$\frac{1}{s}e^{-a/s}$
$\frac{1}{\sqrt{\pi t}}\cos 2\sqrt{at}$	$\frac{1}{\sqrt{s}}e^{-a/s}$
$\frac{1}{\sqrt{\pi t}}\cosh 2\sqrt{at}$	$\frac{1}{\sqrt{s}}e^{a/s}$
$\frac{1}{\sqrt{\pi a}}\sin 2\sqrt{at}$	$\frac{1}{s^{3/2}}e^{-a/s}$
$\frac{1}{\sqrt{\pi a}}\sinh 2\sqrt{at}$	$\frac{1}{s^{3/2}}e^{a/s}$
$I_0(t)$	$\frac{1}{\sqrt{s^2-1}}$

Function	Laplace Transform
$I_n(t)$	$\frac{(s - \sqrt{s^2 - 1})^n}{\sqrt{s^2 - 1}}$
$\frac{a}{2\sqrt{\pi t^3}} e^{-a^2/4t}$	$e^{-a\sqrt{s}} \quad (a > 0)$
$\operatorname{erfc} \frac{a}{2\sqrt{t}}$	$\frac{1}{s} e^{-a\sqrt{s}} \quad (a \geq 0)$
$\frac{1}{\sqrt{\pi t}} e^{-a^2/4t}$	$\frac{1}{\sqrt{s}} e^{-a\sqrt{s}} \quad (a \geq 0)$
$-C - \ln t$	$\frac{1}{s} \ln s$
$\frac{t^{n-1}}{(n-1)!} [\psi(n) - \ln t]$	$\frac{1}{s^n} \ln s \quad (n > 0)$
$E_1(t)$	$\frac{1}{s} \ln(1 + s)$
$\frac{1}{t} (e^{-at} - e^{-bt})$	$\ln \frac{s+b}{s+a}$
$\operatorname{Si}(t)$	$\frac{1}{s} \tan^{-1} \left(\frac{1}{s} \right)$
$\operatorname{Ci}(t)$	$-\frac{1}{2s} \ln(1 + s^2)$
$f(t) \quad (= f(t+T))$	$\frac{\int_0^T e^{-st} f(t) dt}{1 - e^{-sT}}$
Square wave function	$\frac{1}{s} \tanh \frac{1}{4} sT$

Function	Laplace Transform
$f(t_1, t_2)$	$\bar{f}(s_1, s_2)$
$f(t_1)f(t_2)$	$\bar{f}(s_1)\bar{f}(s_2)$
$e^{-\alpha t_1 - \beta t_2} f(t_1, t_2)$	$f(s_1 + \alpha, s_2 + \beta)$
$t_1^m t_2^n f(t_1, t_2)$	$(-1)^{m+n} \frac{\partial^{m+n}}{\partial s_1^m \partial s_2^n} \bar{f}(s_1, s_2)$
$\int_0^{t_1} \int_0^{t_2} f(t_1 - \xi_1, t_2 - \xi_2) g(\xi_1, \xi_2) d\xi_1 d\xi_2$	$\bar{f}(s_1, s_2) \bar{g}(s_1, s_2)$
1	$\frac{1}{s_1 s_2}$
$\sin t_1$	$\frac{1}{s_2(s_1^2 + 1)}$
$\cos t_1 \cos t_2$	$\frac{s_1 s_2}{(s_1^2 + 1)(s_2^2 + 1)}$
$\sin(t_1 + t_2)$	$\frac{s_1 + s_2}{(s_1^2 + 1)(s_2^2 + 1)}$
$e^{\min(t_1, t_2)}$	$\frac{s_1 + s_2}{s_1 s_2 (s_1 + s_2 - 1)}$

11.1.1 Table of z-Transforms

Function	z – Transform
$f(n)$	$F(z) = \sum_{n=0}^{\infty} f(n)z^{-n}$
$f(m) = k; f(n) = 0, n \neq m$	kz^{-n}
k	$\frac{kz}{z - 1}$
kn	$\frac{kz}{(z - 1)^2}$
kn^2	$\frac{kz(z + 1)}{(z - 1)^3}$
α^n	$\frac{z}{z - \alpha}$
$n\alpha^n$	$\frac{\alpha z}{(z - \alpha)^2}$
$\frac{\alpha^n}{n!}$	$e^{\alpha/z}$
$f(n + m), m \geq 1$	$z^m F(z) - z^m f(0) - z^{m-1} f(1) - \cdots - z f(m - 1)$
$a^n f(n)$	$F(z/a)$
$nf(n)$	$-z \frac{d}{dz} F(z)$
$\sum_{k=0}^n f(k)$	$\frac{zF(z)}{z - 1}$
$\sum_{k=0}^n f_2(k)f_1(n - k)$	$F_1(z)F_2(z)$

11.2 The Fast Fourier Transform (FFT)

A classical problem in Mathematics is to determine an approximation to a continuous function $f(x)$ which is of the form

$$f(x) = \frac{1}{2}a_0 + \sum_{r=1}^m (a_r \cos rx + b_r \sin rx), \quad 0 \leq x \leq 2\pi. \quad (11.1)$$

This is equivalent to the interpolation problem of determining the phase polynomial, for appropriate N ,

$$p(x) = \sum_{j=0}^{N-1} \alpha_j e^{ijx}, \quad i = \sqrt{-1}, \quad (11.2)$$

such that

$$p(x_k) = f(x_k), \quad x_k = 2\pi k/N, \quad k = 0, \dots, N-1, \quad (11.3)$$

and it is known that $p(x)$ is uniquely determined by taking

$$\alpha_j = \frac{1}{N} \sum_{k=0}^{N-1} f_k e^{-2\pi ijk/N}, \quad j = 0, \dots, N-1. \quad (11.4)$$

As each α_j requires $O(N)$ multiplications to be evaluated this means that $O(N^2)$ would be needed to evaluate $p(x)$ and, for large values of N , such as would be required to get a discrete representation of the Fourier transform

$$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt, \quad (11.5)$$

this would be challenging for most computers. However, Cooley and Tukey discovered an algorithm which enables (11.2) to be evaluated, for special values of N , in $O(N \log N)$ multiplications. The most straightforward case is where $N = 2^n$.

Suppose $N = 2M$. Then we can find an interpolating polynomial $q(x)$ with the property that

$$q(x_{2s}) = f_{2s}, \quad s = 0, \dots, M-1,$$

and a polynomial $r(x)$ with the property that

$$r(x_{2s+1}) = f_{2s+1}, \quad s = 0, \dots, M-1.$$

Then $p(x)$ can be expressed in terms of the two lower degree phase polynomials by

$$p(x) = q(x) \left(\frac{1 + e^{iMx}}{2} \right) + r(x) \left(\frac{1 - e^{iMx}}{2} \right), \quad (11.6)$$

as when

$$x = x_{2s}, \quad e^{iMx} = e^{iM2\pi(2s)/2M} = e^{2\pi is} = 1,$$

giving

$$p(x_{2s}) = q(x_{2s}) = f_{2s},$$

and when

$$x = x_{2s+1}, \quad e^{iMx} = e^{iM2\pi(2s+1)/2M} = e^{i\pi} = -1,$$

giving

$$p(x_{2s+1}) = r(x_{2s+1}) = f_{2s+1},$$

so that $p(x)$ is the phase polynomial which agrees with $f(x)$ at the interpolation points x_0, \dots, x_{2M-1} .

Equation (11.6) provides the key to the algorithm of Cooley and Tukey which operates in n steps. Step m consists of determining R phase polynomials

$$p_r^{(m)}(x) = \alpha_{r0}^{(m)} + \alpha_{r1}^{(m)} e^{ix} + \dots + \alpha_{r,2M-1}^{(m)} e^{i(2M-1)x}, \quad r = 0, \dots, R-1,$$

from $2R$ phase polynomials $p_r^{(m-1)}(x)$, $r = 0, \dots, 2R-1$ using the identity (11.6), i.e.,

$$2p_r^{(m)}(x) = p_r^{(m-1)}(x)(1 + e^{iMx}) + p_{R+r}^{(m-1)}(x)(1 - e^{iMx}),$$

where $M = 2^{m-1}$, $R = 2^{n-m}$. This gives rise to the recursive relationship between the coefficients of the phase polynomials, namely

$$\left. \begin{aligned} 2\alpha_{rj}^{(m)} &= \alpha_{rj}^{(m-1)} + \alpha_{R+r,j}^{(m-1)} \eta_m^j, & r = 0, \dots, R-1 \\ 2\alpha_{r,M+j}^{(m)} &= \alpha_{rj}^{(m-1)} - \alpha_{R+r,j}^{(m-1)} \eta_m^j, & j = 0, \dots, M-1 \end{aligned} \right\} \quad (11.7)$$

where $\eta = e^{-2\pi i/2^m}$, $m = 0, \dots, n$. The required starting values are

$$\alpha_{k0}^{(0)} = f_k, \quad k = 0, \dots, N-1$$

and, finally, we have $\alpha_j = \alpha_{0j}^{(n)}$, $j = 0, \dots, N-1$.

To summarise, what the FFT enables us to do is, given

$$X(j) = \frac{1}{N} \sum_{k=0}^{N-1} A(k) \exp\left(\frac{2\pi i}{N} jk\right), \quad (11.8)$$

we can determine $A(k)$ from

$$A(k) = \sum_{j=0}^{N-1} X(j) \exp\left(\frac{-2\pi i}{N} jk\right) \quad (11.9)$$

Symbolically we can write this as

$$\{X(j)\} \xrightarrow{FFT} \{A(k)\}. \quad (11.10)$$

11.2.1 Fast Hartley Transforms (FHT)

The discrete Hartley transform pairs are given by the formulae

$$H(j) = \frac{1}{N} \sum_{k=0}^{N-1} h(k) \text{cas}(2\pi jk/N), \quad (11.11)$$

and

$$h(k) = \sum_{j=0}^{N-1} H(j) \text{cas}(2\pi jk/N), \quad (11.12)$$

where $\text{cas}(2\pi jk/N) \equiv \cos(2\pi jk/N) + \sin(2\pi jk/N)$. Here again we can symbolically write

$$\{H(j)\} \xrightarrow{\text{FHT}} \{h(k)\}. \quad (11.13)$$

Note the similarities between this and the discrete Fourier transform pairs (11.8), (11.9). In particular, if N is taken to be a power of 2 then only $N \log N$ operations are required to determine the discrete Hartley transform of a N -point data set.

If real $A(k) = h(k)$ for $i = 0, 1, \dots, N-1$, then $X(j)$ and $H(j)$ are related by

$$\Re\{X(j)\} = \frac{1}{2}(H(j) + H(N-j)), \quad (11.14)$$

and

$$\Im\{X(j)\} = \frac{1}{2}(H(j) - H(N-j)). \quad (11.15)$$

Thus by setting

$$H(j) = \Re\{X(j)\} + \Im\{X(j)\}, \quad j = 0, 1, \dots, \frac{1}{2}N - 1 \quad (11.16)$$

$$H(N-j) = \Re\{X(j)\} - \Im\{X(j)\}, \quad j = 0, 1, \dots, \frac{1}{2}N - 1 \quad (11.17)$$

we can apply the FHT technique. The advantage of using Hartley transforms is that one only needs to use real arithmetic operations in order to determine $h(k)$, since $H(j)$ and $\text{cas}(2\pi jk/N)$ are real, and there is a speed gain (over FFT) as a result.

11.3 Quadrature Rules

Since the inverse Laplace transform is given by an integral, in the Bromwich formulation, it will come as no surprise that the numerical evaluation of integrals plays a big part in numerical methods for the inversion of the Laplace transform. We list here various formulae which we shall require at some stage in developing the techniques described in the book.

The Trapezium Rule

$$\int_a^b f(x)dx = h \sum_{r=0}^n {}''f(a + rh) - \frac{nh^3}{12} f''(\xi) = T_n - \frac{nh^3}{12} f''(\xi), \quad (11.18)$$

where $a < \xi < b$ and $h = (b - a)/n$. The double prime in the summation indicates that the first and last terms in the summation are to be multiplied by the factor $1/2$. We shall sometimes use the notation $T(h)$ instead of T_n to indicate the trapezium rule approximation. It is worth noting that $T(\frac{1}{2}h)$ incorporates function values which have been used in evaluating $T(h)$. In fact we have the identity

$$T(\tfrac{1}{2}h) = (1/2)[T(h) + h \sum_{i=1}^n f(a + (i - \tfrac{1}{2})h)]. \quad (11.19)$$

A disadvantage of the trapezium rule is that it breaks down if the integrand has a singularity at the end point. This can be overcome by using a modified trapezium rule formula (see Cohen [43]) with the appropriate Richardson extrapolation expansion — see Sidi [216] for a detailed discussion of Richardson extrapolation. The rule is sometimes referred to as the trapezoidal rule.

The Euler-Maclaurin Summation Formula

$$\begin{aligned} \int_a^b f(x)dx &= T_n - \frac{B_2}{2!} h^2 [f'(b) - f'(a)] - \dots \\ &\quad - \frac{B_{2k} h^{2k}}{(2k)!} [f^{(2k-1)}(b) - f^{(2k-1)}(a)] + R_{2k}, \end{aligned} \quad (11.20)$$

where T_n is defined as in (11.18), B_{2k} denote the Bernoulli numbers and

$$R_{2k} = \frac{\theta_n B_{2k+2} h^{2k+3}}{(2k+2)!} \max_{a \leq x \leq b} |f^{(2k+2)}(x)|, \quad -1 \leq \theta \leq 1.$$

Although, in many applications of the trapezium rule, the truncation error can be quite large it is clear from the Euler - Maclaurin summation formula that where the odd order derivatives tend to zero at the end-points this rule can be very successful.

Example 11.1 Evaluate $\int_{-\infty}^{\infty} e^{-x^2} dx$.

We have the results in Table 11.1 .

Note that as the integrand is $O(10^{-44})$ for $x = \pm 10$ we have taken $a = -10$ and $b = 10$ and clearly we have converged rapidly to the correct answer of $\sqrt{\pi}$.

The Mid-point Rule

$$\int_a^b f(x)dx = h \sum_{k=1}^n f(a + (k - \tfrac{1}{2})h) + \frac{nh^3}{24} f''(\xi) = M_n + \frac{nh^3}{24} f''(\xi), \quad (11.21)$$

h	$T(h)$
1.0	1.7726372048...
0.5	1.77245385090551605266...
0.25	1.77245 38509 05516 02729 81674 83341
0.125	1.77245 38509 05516 02729 81674 83341

Table 11.1: Evaluation of $\int_{-\infty}^{\infty} e^{-x^2} dx$ by the trapezium rule.

where $a < \xi < b$ and $h = (b - a)/n$. One of the disadvantages of using the mid-point rule is that a completely new set of function values has to be computed if we are comparing estimates for the integral for any two values of n . An advantage of the mid-point rule is that it can be used to estimate integrals where there is a singularity at an end point.

Gaussian Quadrature Rules

These take the form

$$\int_a^b w(x)f(x)dx = \sum_{k=1}^n \alpha_k f(x_k) + R_n, \quad (11.22)$$

where $w(x)$ is a positive weight function in (a, b) , the $\{x_k\}$ denote the roots of the equation $p_n(x) = 0$, where the polynomials $\{p_n(x)\}$ satisfy the orthogonality relationships

$$\int_a^b w(x)p_m(x)p_n(x)dx = 0, \quad m \neq n \quad (11.23)$$

$$= \gamma_n, \quad m = n \quad (11.24)$$

and the $\{\alpha_k\}$ are constants, known as Christoffel numbers, given by

$$\alpha_k = -\frac{A_{n+1}\gamma_n}{A_n p'_n(x_k)p_{n+1}(x_k)}, \quad (11.25)$$

where A_n is the coefficient of x^n in $p_n(x)$ and, finally, the remainder term R_n is given by

$$R_n = \frac{\gamma_n}{A_n^2} \cdot \frac{f^{(2n)}(\xi)}{(2n)!}, \quad a < \xi < b. \quad (11.26)$$

Thus, in the case where $w(x) = 1$ and $[a, b] = [-1, 1]$ we have the Gauss-Legendre quadrature formula

$$\int_{-1}^1 f(x)dx = \sum_{k=1}^n \alpha_k f(x_k) + R_n, \quad (11.27)$$

where

$$R_n = \frac{2^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\xi), \quad -1 < \xi < 1 \quad (11.28)$$

$$\alpha_k = 2/(1 - x_k^2)[P'_n(x_k)]^2, \quad (11.29)$$

$\{x_k\}$, $k = 1, \dots, n$ are the roots of the equation $P_n(x) = 0$ and $P_n(x)$ is the n^{th} degree Legendre polynomial.

When $w(x) = 1/\sqrt{1-x^2}$ and $[a, b] = [-1, 1]$ we have the Gauss-Chebyshev quadrature formula

$$\int_{-1}^1 \frac{f(x)}{\sqrt{1-x^2}} dx = \frac{\pi}{n} \sum_{k=1}^n f(x_k) + R_n, \quad x_k = \cos \frac{(2k-1)\pi}{2n}, \quad (11.30)$$

where

$$R_n = \frac{\pi}{(2n)!2^{2n-1}} f^{(2n)}(\xi), \quad -1 < \xi < 1. \quad (11.31)$$

We give one more example with $w(x) = e^{-x}$ and $[a, b] = [0, \infty)$. The related orthogonal polynomials in this case are the Laguerre polynomials $L_n(x)$. The abscissae x_k are roots of $L_n(x) = 0$ and the weights satisfy

$$\alpha_k = \frac{(n!)^2 x_k}{(n+1)^2 [L_{n+1}(x_k)]^2}, \quad (11.32)$$

giving the Gauss-Laguerre quadrature formula

$$\int_0^\infty e^{-x} f(x) dx = \sum_{k=1}^n \alpha_k f(x_k) + R_n, \quad (11.33)$$

where the remainder R_n satisfies

$$R_n = \frac{(n!)^2}{(2n)!} f^{(2n)}(\xi), \quad 0 < \xi < \infty. \quad (11.34)$$

Change of Interval and Integration Strategies

The substitution $y = \frac{1}{2}(b-a)x + \frac{1}{2}(b+a)$, where a and b are finite, converts the integration range from $[a, b]$ to $[-1, 1]$. We have

$$\int_a^b f(y) dy = \frac{1}{2}(b-a) \int_{-1}^1 f\left[\frac{1}{2}(b-a)x + \frac{1}{2}(b+a)\right] dx. \quad (11.35)$$

The integral on the right hand side can be estimated by means of a Gauss-Legendre formula.

In practice it is not always possible to determine the truncation error R_n explicitly. Possible strategies for ensuring accuracy are:-

(1) Compare estimates for the integral using n , $n + 1$ and $n + 2$ point formulae.

(2) Use an adaptive approach. We determine an estimate for the integral with a n -point formula. Since

$$\int_{-1}^1 f(x)dx = \int_{-1}^0 f(x)dx + \int_0^1 f(x)dx,$$

we can obtain another estimate by evaluating each of the right hand side integrals using the same n -point formula. We then compare estimates and subdivide the interval again if necessary.

(3) Estimate with a n -point formula and by judicious choice of extra abscissae make a revised estimate for the integral — this is known as Gauss-Kronrod integration. The reader should consult Davis and Rabinowitz [61] or Evans [81] for further details.

The method of Clenshaw and Curtis

This method for evaluating

$$\int_{-1}^1 f(x)dx,$$

assumes that $f(x)$ is continuous and differentiable and has an expansion in Chebyshev polynomials, i.e.

$$f(x) \approx \sum_{k=0}^N {}''a_k T_k(x), \quad (11.36)$$

where the double prime indicates that the first and last terms of the summation are to be halved and $T_k(x)$ denotes the Chebyshev polynomial of degree k . Since

$$\int T_n(x)dx = \frac{1}{2} \left(\frac{T_{n+1}(x)}{n+1} - \frac{T_{n-1}(x)}{n-1} \right), \quad n > 1$$

it follows that

$$\int_{-1}^1 f(x)dx = 2(C_1 + C_3 + C_5 + \cdots), \quad (11.37)$$

where

$$C_r = \frac{1}{2r}(a_{r-1} - a_{r+1}), \quad r = 1, 2, \dots, N-1$$

$$C_N = a_{N-1}/2N, \quad C_{N+1} = a_N/2(N+1).$$

O'Hara and Smith [162] have proposed a bound for the error in the Clenshaw-Curtis method, namely

$$|E_N| < \max\{2|a_{N-4}|, 2|a_{N-2}|, |a_N|\}. \quad (11.38)$$

This is not entirely foolproof and it is advisable to compare with calculations obtained for larger N .

Oscillatory Integrands

There are many situations where we have a solution to a problem in the form

$$I = \int_a^b f(x)w(x)dx, \quad (11.39)$$

where, typically,

$$w(x) = \cos \omega x \quad \text{or} \quad \sin \omega x \quad \text{or} \quad J_0(\omega x), \quad (11.40)$$

and $J_0(x)$ is the Bessel function of the first kind of zero order, $f(x)$ is a smooth function and ω is a fairly large positive constant. The range $[a, b]$ could be finite but may be $[0, \infty)$. In the case $[a, b]$ finite and $w(x) = \sin \omega x$, Filon [84] divided the range of integration into $2n$ equal parts and, in each sub-interval of width $2h$ where $b = a + 2nh$, approximated $f(x)$ by a quadratic polynomial. He thus obtained

$$\int_a^b f(x) \sin \omega x dx = h[\alpha\{f(a) \cos \omega a - f(b) \cos \omega b\} + \beta S_{2n} + \gamma S_{2n-1}], \quad (11.41)$$

where

$$S_{2n} = \frac{1}{2}[f(a) + f(b)] + \sum_{k=1}^{n-1} f(x_{2k}), \quad (11.42)$$

$$S_{2n-1} = \sum_{k=1}^n f(x_{2k-1}), \quad (11.43)$$

and

$$\begin{aligned} \alpha &= \frac{1}{\theta} + \frac{\cos \theta \sin \theta}{\theta^2} - \frac{2 \sin^2 \theta}{\theta^3}, \\ \beta &= 2 \left(\frac{1 + \cos^2 \theta}{\theta^2} - \frac{2 \sin \theta \cos \theta}{\theta^3} \right), \\ \gamma &= 4 \left(\frac{\sin \theta}{\theta^3} - \frac{\cos \theta}{\theta^2} \right), \quad \text{where } \theta = \omega h. \end{aligned}$$

Estimates for the error in Filon's method are given in Abramowitz and Stegun [5]. Evans [81] gives a detailed treatment of recent advances. Most methods seem to have drawbacks of some sort — numerical instability being a particular problem — but, overall, Evans seems to favour Patterson's method [166] which uses Gauss-Kronrod integration. This approach is available as NAG Library Routine D01AKF.

Infinite Integrals

If $f(t)$ is a monotone decreasing function of t then, since

$$\int_0^\infty f(t)dt = \int_0^1 f(t)dt + \int_1^2 f(t)dt + \cdots,$$

we can treat this as a series summation problem with

$$a_r = \int_{r-1}^r f(t)dt,$$

and use the extrapolation methods given in the next section to determine the sum of the series and hence the integral. More generally, we can write

$$\int_0^\infty f(t)dt = \int_{t_0}^{t_1} f(t)dt + \int_{t_1}^{t_2} f(t)dt + \cdots,$$

where $0 = t_0 < t_1 < t_2 < \cdots$ is some appropriate subdivision of the real axis.

If the integrand is of oscillatory type, as in (11.39), then by choosing $t_0 = 0$ and t_i to be the i th consecutive point at which $w(t)$ is zero we have

$$\begin{aligned} \int_0^\infty f(t)w(t)dt &= \int_{t_0}^{t_1} f(t)w(t)dt + \int_{t_1}^{t_2} f(t)w(t)dt + \int_{t_2}^{t_3} f(t)w(t)dt + \cdots, \\ &= a_1 - a_2 + a_3 - \cdots, \end{aligned}$$

where

$$a_r = (-1)^{r-1} \int_{t_{r-1}}^{t_r} f(t)w(t)dt,$$

is a positive quantity. We can employ the methods of the next section to sum the alternating series. See §4.3 where this technique has been applied.

11.4 Extrapolation Techniques

In this section we collect together a number of extrapolation methods which have been used by various authors who have developed methods for the numerical inversion of Laplace transforms and which have been quoted in earlier chapters. It is worth pointing out at this stage that an extrapolation method is only guaranteed to work if the sequence it is applied to satisfies the conditions which were imposed in its construction. This is rarely known *ab initio* and it may require some difficult mathematics to establish the linkage. It is precisely because of these difficulties that we have advocated the use of at least two different methods in order to establish the inverse Laplace transform.

More details about these and other methods, which should not be ignored, can

be found in the books by Brezinski and Redivo-Zaglia [25] and Sidi [216].

Euler's method of summation for Alternating Series

Given a convergent series

$$s = xv_1 - x^2v_2 + x^3v_3 - \cdots + (-1)^{n-1}v_n + \cdots, \quad 0 < x < 1, \quad (11.44)$$

we can make the substitution $x = y/(1 - y)$ to give, after expansion and rearrangement,

$$s = yv_1 - y^2\Delta v_1 + y^3\Delta^2v_1 - \cdots + y^n(-\Delta)^{n-1}v_1 + \cdots, \quad (11.45)$$

where $\Delta^r v_1$ has its usual meaning

$$\Delta^r v_1 = v_{r+1} - \binom{r}{1}v_r + \binom{r}{2}v_{r-1} - \cdots + (-1)^{r-1}\binom{r}{r-1}v_2 + (-1)^r v_1.$$

In particular, when $x = 1$, we have the result

$$\begin{aligned} s &= v_1 - v_2 + v_3 - \cdots + (-1)^{n-1}v_n + \cdots \\ &= \frac{1}{2}v_1 - \frac{1}{4}\Delta v_1 + \frac{1}{8}\Delta^2v_1 - \cdots + \frac{1}{2^n}(-\Delta)^{n-1}v_1 + \cdots \\ &= \frac{1}{2} \sum_1^\infty \left(-\frac{1}{2}\Delta\right)^{n-1} v_1. \end{aligned} \quad (11.46)$$

In practical applications a well-tried strategy is to write

$$s = s_1 + s_2, \quad \text{where} \quad s_1 = v_1 - v_2 + \cdots + (-1)^{k-1}v_k,$$

and to sum s_1 directly and apply the Euler summation formula (11.46) to evaluate s_2 — if $x \neq 1$ the same strategy can be used in conjunction with (11.45). The Euler summation formula can also be used to find the sum of divergent series which are summable in the Cesaro sense.

Hutton's method for Alternating Series

If s_n denotes the partial sums of an alternating series then if we define

$$s_{-1}^{(k)} = 0 \quad (k \geq 0), \quad s_n^{(0)} = s_n \quad (n \geq 0),$$

with

$$s_n^{(k)} = \frac{1}{2}(s_{n-1}^{k-1} + s_n^{k-1}) \quad (n \geq 0), \quad (11.47)$$

we have an algorithm which enables us to determine s . Here also we can determine s if the series is divergent but summable in the Cesaro sense.

The iterated Aitken method for Alternating Series

This method is based on the result that if a sequence $\{x_n\}$ has the property that

$$x_n = x + Ar^n,$$

k	$S_1^{(k)}$
3	0.69314887
4	0.693147196
5	0.69314718066
6	0.693147180560
7	0.693147180559944
8	0.693147180559943

Table 11.2: Summation of $\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n}$ by iterated Aitken method.

where A, r and x are constants then, given three consecutive terms x_n, x_{n+1} and x_{n+2} , we have

$$x = x_{n+2} - \frac{(x_{n+2} - x_{n+1})^2}{x_{n+2} - 2x_{n+1} + x_n}.$$

To apply this to the summation of alternating series we compute the partial sums of the series $S_1^{(0)}, S_2^{(0)}, \dots, S_{2k+1}^{(0)}$ and for three consecutive entries $S_j^{(r)}, S_{j+1}^{(r)}, S_{j+2}^{(r)}$ ($r = 0, 1, 2, \dots$) we form

$$S_j^{(r+1)} = S_j^{(r)} - \frac{(S_j^{(r)} - S_{j+1}^{(r)})^2}{S_j^{(r)} - 2S_{j+1}^{(r)} + S_{j+2}^{(r)}}, \quad (11.48)$$

and proceed with calculations until we eventually arrive at $S_1^{(k)}$.

Example 11.2 Estimate the sum of the series $S = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \dots$.

We obtain the results in Table 11.2

See Cohen [44] for a derivation of the method and Sidi [216] regarding convergence properties.

The Shanks Transformation

Assume that a sequence $\{A_n\}$ has behaviour of the form

$$A_r = C_{kn} + \sum_{i=1}^k \alpha_{in}(r) f_i(r), \quad (11.49)$$

and r is bounded appropriately. In the case where $\alpha_{in}(r) = \alpha_i \neq 0$, $f_i(r) = q_i^r$, $n - k \leq r \leq n + k$ and $C_{kn} = S_{kn}$ we have the Shanks transformation [208]

which can be expressed in terms of determinants by Cramer's rule, namely,

$$S_{kn} = \frac{\begin{vmatrix} A_{n-k} & \cdots & A_{n-1} & A_n \\ \Delta A_{n-k} & \cdots & \Delta A_{n-1} & \Delta A_n \\ \vdots & \cdots & \vdots & \vdots \\ \Delta A_{n-1} & \cdots & \Delta A_{n+k-2} & \Delta A_{n+k-1} \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 & 1 \\ \Delta A_{n-k} & \cdots & \Delta A_{n-1} & \Delta A_n \\ \vdots & \cdots & \vdots & \vdots \\ \Delta A_{n-1} & \cdots & \Delta A_{n+k-2} & \Delta A_{n+k-1} \end{vmatrix}} \quad (11.50)$$

where $A_r = A_{r+1} - A_r$. S_{kn} is identical with the $[k/n]$ Padé approximant of the series

$$A_1 + \sum_{j=1}^{\infty} (\Delta A_j) z^j \quad (11.51)$$

evaluated at $z = 1$.

The ϵ -algorithm

Wynn [257] found that the term S_{kn} in the Shanks transformation could be obtained in an efficient way by means of the ϵ -algorithm, namely,

$$\left. \begin{aligned} \epsilon_{-1}^{(n)} &= 0, & \epsilon_0^{(n)} &= A_n \\ \epsilon_{k+1}^{(n)} &= \epsilon_{k-1}^{(n+1)} + \frac{1}{\epsilon_k^{(n+1)} - \epsilon_k^{(n)}} \end{aligned} \right\} \quad k, n = 0, 1, \dots \quad (11.52)$$

yielding

$$\epsilon_{2k}^{(n)} = S_{k, n+k}, \quad k, n = 0, 1, \dots \quad (11.53)$$

The Levin t- and u- transformations

If, in (11.49), we take $\alpha_{in}(r) = \alpha_{in} R_r$, $n \leq r \leq n+k$ and $C_{kn} = T_{kn}$ then application of Cramer's rule gives

$$T_{kn} = \frac{\begin{vmatrix} A_n & A_{n+1} & \cdots & A_{n+k} \\ R_n f_0(n) & R_{n+1} f_0(n+1) & \cdots & R_{n+k} f_0(n+k) \\ \vdots & \vdots & \cdots & \vdots \\ R_n f_{k-1}(n) & R_{n+1} f_{k-1}(n+1) & \cdots & R_{n+k} f_{k-1}(n+k) \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \cdots & 1 \\ R_n f_0(n) & R_{n+1} f_0(n+1) & \cdots & R_{n+k} f_0(n+k) \\ \vdots & \vdots & \cdots & \vdots \\ R_n f_{k-1}(n) & R_{n+1} f_{k-1}(n+1) & \cdots & R_{n+k} f_{k-1}(n+k) \end{vmatrix}} \quad (11.54)$$

By making the assumption that each $R_r \neq 0$ it is possible to divide column j of each determinant by R_{n+j-1} . The choice

$$f_i(r) = 1/r^i$$

k	u_{k1}
6	1.64493519
8	1.6449340412
10	1.64493406715
12	1.64493406684718
14	1.64493406684819
16	1.6449340668482275
18	1.64493406684822642

Table 11.3: Summation of $\sum_{n=1}^{\infty} \frac{1}{n^2}$ by Levin's method.

then enables us to express the determinants in terms of Vandermonde determinants and we obtain

$$T_{kn} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k} \right)^{k-1} \frac{A_{n+j}}{R_{n+j}}}{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k} \right)^{k-1} \frac{1}{R_{n+j}}}. \quad (11.55)$$

We have not specified the R_r . Levin [126] made the choice $R_r = \Delta A_{r-1}$ as the most appropriate for the summation of alternating series where the A_r are the partial sums of the series (the Levin t -transformation). The choice $R_r = r\Delta A_{r-1}$ gives the Levin u -transformation

$$U_{kn} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k} \right)^{k-2} \frac{A_{n+j}}{R_{n+j}}}{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{n+j}{n+k} \right)^{k-2} \frac{1}{R_{n+j}}}, \quad (11.56)$$

which Levin used for the summation of positive series. We now give some examples of the application of the t - and u -transformations. Because of cancellation increasing the number of terms used in the u -transformation might lead to numerical instability. When applying the t -transformation to summing alternating series cancellation is not a problem (as all terms are positive) but it is important to add terms in the numerator and denominator in increasing order of magnitude.

Example 11.3 Find the sum of the series $S = \sum_{k=1}^{\infty} 1/n^2$.

This is an example given by Levin [126] and the exact answer is well-known to be $\pi^2/6 = 1.644934066848226436 \dots$. Applying formula (11.56), with $n = 1$, we obtained the results in Table 11.3.

The next example gives an illustration of how the t -transform can be applied to estimate the sum of a divergent series.

Example 11.4 Find the sum of the series $1 - 1! + 2! - 3! + 4! - \dots$.

This divergent series arises when trying to compute

$$I = \int_0^{\infty} \frac{e^{-t} dt}{1+t},$$

k	$t_{k1}(S)$
6	0.59633059
8	0.59634941
10	0.59634720
12	0.59634737
14	0.5963473617
16	0.596347362335
18	0.596347362327
20	0.596347362322

Table 11.4: Summation of $\sum_{n=0}^{\infty} (-1)^n n!$ by the Levin t -transform.

and one assumes that

$$\frac{1}{1+t} = 1 - t + t^2 - t^3 + \cdots .$$

Substitution into the integrand gives

$$I = 1 - 1! + 2! - 3! + 4! - \cdots .$$

The exact value of I is $eE_1(1)$ where $E_1(x)$ is the exponential integral, see Abramowitz and Stegun [5]. Application of (11.55) provides a good estimate as k increases as we see from Table 11.4 . The Levin t -transform can be used to estimate the sum (also called anti-limit) of other divergent series which converge in the Cesaro sense.

The S -transformation of Sidi

This is more effective than the Levin t -transform and has better convergence properties with regard to the summation of everywhere divergent series . If we assume that the sequence $\{A_n\}$ has behaviour of the form

$$A_r = S_{kn} + R_r \sum_{i=0}^{n-1} \frac{\alpha_i}{(r)_i}, \quad (11.57)$$

where $(n)_0 = 1$ and $(n)_i = n(n+1) \cdots (n+i-1)$, $i = 1, 2, \cdots$ is the Pochhammer symbol . We can obtain a closed form expression for this transformation, namely

$$S_{kn} = \frac{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{(n+j)_{k-1}}{(n+k)_{k-1}} \right) \frac{A_{n+j}}{R_{n+j}}}{\sum_{j=0}^k (-1)^j \binom{k}{j} \left(\frac{(n+j)_{k-1}}{(n+k)_{k-1}} \right) \frac{1}{R_{n+j}}}, \quad R_r = \Delta A_{r-1}. \quad (11.58)$$

We now apply the Sidi S -transform to estimate the sum of the divergent series given in the previous example.

Example 11.5 Find the sum of the series $1 - 1! + 2! - 3! + 4! - \cdots$.

Application of (11.58) yields Table 11.5. The reader should compare the results in Table 11.5 with those in Table 11.4.

k	S_{k1}
6	0.59634724
8	0.596347768
10	0.5963473531
12	0.5963473608
14	0.59634736236
16	0.5963473623346
18	0.5963473623233
20	0.59634736232308

Table 11.5: Summation of $\sum_{n=0}^{\infty} (-1)^n n!$ by the Sidi S -transform**The Levin-Sidi $d^{(m)}$ -transformation**

This is a more general transformation than the Levin t - and u -transformations and includes them as special cases. Briefly, let the sequence $\{A_n\}$ be such that $a_n = A_n - A_{n-1}$, $n = 1, 2, \dots$, satisfy a linear m th order difference equation of the form

$$a_n = \sum_{k=1}^m p_k(n) \Delta a_n,$$

where

$$p_k(n) \sim n^{i_k} \left(\alpha_{k0} + \frac{\alpha_{k1}}{n} + \frac{\alpha_{k2}}{n^2} + \dots \right), \quad \text{as } n \rightarrow \infty,$$

and i_k are integers satisfying $i_k \leq k$, $k = 1, \dots, m$. Subject to certain conditions holding, Levin and Sidi show that $\sum_{i=n}^{\infty} a_i$ has an asymptotic expansion of the form

$$\sum_{i=n}^{\infty} a_i \sim \sum_{k=0}^{m-1} n_k^{\rho} (\Delta^k a_n) \left(\beta_{k0} + \frac{\beta_{k1}}{n} + \frac{\beta_{k2}}{n^2} + \dots \right), \quad \text{as } n \rightarrow \infty,$$

where

$$\rho_k \leq \max(i_{k+1}, i_{k+2} - 1, \dots, i_m - m + k + 1), \quad k = 0, 1, \dots, m-1.$$

Based on this asymptotic expansion, the $d^{(m)}$ -transformation is defined as follows:

Choose a sequence of integers $1 \leq R_0 < R_1 < R_2 < \dots$, and let $n = (n_1, \dots, n_m)$, where n_k are nonnegative integers. Then the approximation $d_n^{(m,j)}$ to the sum $\sum_{i=1}^{\infty} a_i$ is defined via the solution of the linear system of equations

$$\sum_{i=1}^{R_l} a_i = d_n^{(m,j)} + \sum_{k=1}^m R_l^{\rho_{k-1}} (\Delta^{k-1} a_{R_l}) \sum_{i=0}^{n_k-1} \frac{\bar{\beta}_{ki}}{R_l^i}, \quad (11.59)$$

$$l = j, j+1, \dots, j+N; \quad N = \sum_{k=1}^m n_k.$$

When the ρ_k are not known, they can be replaced in (11.59) by their upper bounds, namely, by $k + 1$, $k = 0, 1, \dots, m - 1$. Thus, $R_l^{\rho_{k-1}}$ in these equations is replaced by R_l^k .

Note that, the Levin u- and t-transformations are special cases of the $d^{(1)}$ -transformation with $R_l = l + 1$, $l = 0, 1, \dots$. We have $\rho_1 = 0$ for the t-transformation and $\rho_1 = 1$ for the u-transformation.

The sequences of “diagonal” approximations $d_n^{(m,j)}$ with $n = (\nu, \dots, \nu)$, $\nu = 1, 2, \dots$, seem to have the best convergence properties. These approximations can be computed recursively and in an efficient manner via the $W^{(m)}$ -algorithm of Ford and Sidi [86]. A program for this algorithm is given at the website www.cf.ac.uk/maths/cohen/programs/inverselaplacetransform/.

When $m = 1$, the $W^{(m)}$ -algorithm reduces to the W -algorithm of Sidi [213], which, in the present context of the $d^{(1)}$ -transformation, reads as follows:

$$\begin{aligned} M_0^{(j)} &= \frac{A_{R_j}}{\omega_{R_j}}, \quad N_0^{(j)} = \frac{1}{\omega_{R_j}}, \quad j \geq 0; \quad \omega_r = r^\rho a_r, \\ M_n^{(j)} &= \frac{M_{n-1}^{(j+1)} - M_{n-1}^{(j)}}{R_{j+n}^{-1} - R_j^{-1}}, \quad N_n^{(j)} = \frac{N_{n-1}^{(j+1)} - N_{n-1}^{(j)}}{R_{j+n}^{-1} - R_j^{-1}}, \quad j \geq 0, \quad n \geq 1. \\ d_n^{(1,j)} &= \frac{M_n^{(j)}}{N_n^{(j)}}, \quad j, n \geq 0. \end{aligned}$$

Here $\rho = 0$ in the case the series $\sum_{i=1}^{\infty} a_i$ is linearly converging, whether alternating (i.e. $a_i a_{i+1} < 0$ all i) or monotonic (i.e. $a_i > a_{i+1} > 0$ or $a_i < a_{i+1} < 0$ all i), and $\rho = 1$ when this series is logarithmically converging.

The following choices of the integers R_l (see Sidi [216]) have proved to be very effective in obtaining stable approximations of high accuracy in different cases:

1. Arithmetic Progression Sampling (APS)

$$R_l = [\kappa(l + 1)], \quad l = 0, 1, \dots; \quad \text{for some } \kappa \geq 1,$$

where $[x]$ = integer part of x .

2. Geometric Progression Sampling (GPS)

$$R_0 = 1, \quad R_l = \begin{cases} R_{l-1} + 1 & \text{if } [\sigma R_{l-1}] \leq R_{l-1}, \\ [\sigma R_{l-1}] & \text{otherwise,} \end{cases} \quad l = 0, 1, \dots; \quad \text{for some } \sigma > 1.$$

Here are two examples with $m = 1$.

In the case where $\{A_n\}$ is a logarithmically converging sequence, GPS should be used (with $\sigma = 1.3$, for example). An example of this type is $A_n = \sum_{i=1}^n 1/i^2$, whose limit is $\pi^2/6$.

In the case where $\{A_n\}$ is a linearly (but slowly) converging sequence with ΔA_n

of the same sign, APS should be used with $\kappa > 1$. One such sequence of this type is $A_n = -\sum_{i=1}^n x^i/i$, whose limit is $\log(1-x)$. This is the case when $x \lesssim 1$, the point of singularity (branch point) of the limit $\log(1-x)$. For example, $\kappa = 4$ will do for $x = 0.9$, while $\kappa = 6$ will work for $x = 0.95$. ($\kappa = 1$ produces inferior results.) When x is sufficiently far from $x = 1$ (for example, $x = 0.5$ or $x = -1$), $\kappa = 1$ will suffice.

The ρ -algorithm of Wynn

This is given by

$$\begin{aligned}\rho_1^{(n)} &= 0, & \rho_0^{(n)} &= A_n, \\ \rho_{k+1}^{(n)} &= \rho_{k-1}^{(n+1)} + \frac{x_{n+k+1} - x_n}{\rho_k^{(n+1)} - \rho_k^{(n)}}, & k, n &= 0, 1, \dots\end{aligned}\quad (11.60)$$

In the original formulation Wynn [258] takes $x_n = n$. This algorithm has been successfully applied to extrapolate the sequence of results obtained using the Post-Widder and Gaver formulae (see §9.3.4). The ρ -algorithm is only effective when

$$A_n \sim \alpha_0 + \frac{\alpha_1}{n} + \frac{\alpha_2}{n^2} + \dots \quad \text{as } n \rightarrow \infty; \quad \lim_{n \rightarrow \infty} A_n = \alpha_0.$$

It is ineffective in other cases.

As stated at the beginning of this section we have given an account of the extrapolation methods which have been employed in this book. For a comprehensive coverage of extrapolation methods the reader is referred to the books by Brezinski and Redivo-Zaglia [25] and Sidi [216].

11.5 Padé Approximation

Suppose a function $f(z)$ has an expansion

$$f(z) = \sum_{k=0}^{\infty} a_k z^k. \quad (11.61)$$

We would like to approximate $f(z)$ by a rational function $f_{p,q}(z)$ where

$$f_{p,q}(z) = P(z)/Q(z), \quad (11.62)$$

and $P(z)$ and $Q(z)$ are respectively polynomials of degree p and q . If

$$Q(z)f(z) - P(z) = z^{p+q+1}E_{p,q}(z), \quad E_{p,q}(0) \neq 0, \quad (11.63)$$

then (11.62) is called a Padé approximation of $f(z)$. We can think of $f_{p,q}(z)$ as an element of a matrix and when $p = q$ we get the element (p, p) on the main

diagonal. More generally, we say that $f_{p,q}(z)$ occupies the (p, q) position in the Padé table. This is also sometimes referred to as the $[p/q]$ Padé approximant. The Padé approximants to a Taylor series expansion can always be found by solving a system of linear equations. For if

$$P(z) = \sum_{k=0}^p b_k z^k, \quad Q(z) = \sum_{k=0}^q c_k z^k,$$

then comparison of powers of z in (11.63) gives rise to the system of equations

$$\begin{aligned} b_k &= \sum_{j=0}^k a_j c_{k-j}, & k &= 0, \dots, p, \\ \sum_{j=0}^m a_j c_{m-j} &= 0, & m &= p+1, \dots, p+q, \\ E_{p,q}(z) &= \sum_{k=0}^{\infty} e_k z^k, & e_k &= \sum_{j=0}^q c_j a_{p+q+k+1-j}. \end{aligned} \quad (11.64)$$

An alternative expression for $E_{p,q}(z)$ is

$$E_{p,q}(z) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{Q(w)E(w)}{(w-z)^{p+q+1}} dw, \quad (11.65)$$

where the closed contour \mathcal{C} encloses $w = 0$ and $w = z$ and $E(w)$ is analytic within and on \mathcal{C} .

The necessity to solve the systems of equations (11.64) to find the Padé approximants $f_{p,p}(z)$ and $f_{p,p+1}(z)$ can be obviated by using a technique due to Viskovatoff (see Khovanskii [119]). Suppose that a function $g(z)$ has the more general form

$$g(z) = \sum_{k=0}^{\infty} \alpha_{1k} z^k \bigg/ \sum_{k=0}^{\infty} \alpha_{0k} z^k. \quad (11.66)$$

Then

$$\begin{aligned}
 g(z) &= \frac{\alpha_{10}}{\alpha_{00} + z \frac{(\alpha_{10}\alpha_{01} - \alpha_{00}\alpha_{11}) + (\alpha_{10}\alpha_{02} - \alpha_{00}\alpha_{12})z + \cdots}{\alpha_{10} + \alpha_{11}z + \alpha_{12}z^2 + \cdots}} \\
 &= \frac{\alpha_{10}}{\alpha_{00} + z \frac{\alpha_{20} + \alpha_{21}z + \alpha_{22}z^2 + \cdots}{\alpha_{10} + \alpha_{11}z + \alpha_{12}z^2 + \cdots}} \\
 &= \frac{\alpha_{10}}{\alpha_{00} + z \frac{\alpha_{20}}{\alpha_{10} + z \frac{(\alpha_{20}\alpha_{11} - \alpha_{10}\alpha_{21}) + (\alpha_{20}\alpha_{12} - \alpha_{10}\alpha_{22})z + \cdots}{\alpha_{20} + \alpha_{21}z + \alpha_{22}z^2 + \cdots}}} \\
 &= \frac{\alpha_{10}}{\alpha_{00} + \frac{\alpha_{20}z}{\alpha_{10} + \frac{\alpha_{30}z}{\alpha_{20} + \frac{\alpha_{40}z}{\alpha_{30} + \cdots}}}} \tag{11.67}
 \end{aligned}$$

The α_{ij} , $i, j = 0, 1, 2, \dots$ may be thought of as the elements of an infinite matrix and can be computed recursively by the formula

$$\alpha_{rs} = \alpha_{r-1,0}\alpha_{r-2,s+1} - \alpha_{r-2,0}\alpha_{r-1,s+1}. \tag{11.68}$$

Hence given the ratio of two power series (11.66) we can develop the continued fraction (11.67) and by truncation we can obtain the approximations $f_{p,p}(z)$ and $f_{p,p+1}(z)$.

We also mention here Padé-type approximants. If we define $f(z)$ as above by (11.61) and $v(z)$, $w(z)$ respectively by

$$\begin{aligned}
 v(z) &= b_0z^k + b_1z^{k-1} + \cdots + b_k, \\
 w(z) &= c_0z^{k-1} + c_1z^{k-2} + \cdots + c_{k-1},
 \end{aligned}$$

where

$$c_i = \sum_{j=0}^{k-i-1} a_j b_{i+j+1}, \quad i = 0, \dots, k-1$$

then $w(z)/v(z)$ is called the $(k-1/k)$ Padé-type approximation to $f(z)$ and satisfies

$$\frac{w(z)}{v(z)} - f(z) = O(z^k), \quad z \rightarrow 0. \tag{11.69}$$

More general results about Padé approximants, Padé-type approximants and continued fractions (see next section) and the inter-relationship between them can be found in the books by Baker and Graves-Morris [10], Brezinski [24] and Sidi [216].

11.5.1 Continued Fractions. Thiele's method

An expression of the form

$$\frac{a_1}{b_1+} \frac{a_2}{b_2+} \frac{a_3}{b_3+\cdots},$$

is called a continued fraction. The above expression is shorthand notation for

$$\frac{a_1}{b_1 + \frac{a_2}{b_2 + \frac{a_3}{b_3 + \cdots}}}.$$

The n th convergent, denoted by $x_n = p_n/q_n$ is given by

$$x_n = \frac{a_1}{b_1+} \frac{a_2}{b_2+\cdots} \frac{a_n}{b_n},$$

and can be computed by means of the recurrence formulae

$$p_0 = 0, \quad p_1 = a_1, \quad p_k = b_k p_{k-1} + a_k p_{k-2} \quad (k \geq 2), \quad (11.70)$$

$$q_0 = 1, \quad q_1 = b_1, \quad q_k = b_k q_{k-1} + a_k q_{k-2} \quad (k \geq 2). \quad (11.70a)$$

If

$$x = \lim_{n \rightarrow \infty} x_n,$$

exists we write

$$x = \frac{a_1}{b_1+} \frac{a_2}{b_2+} \frac{a_3}{b_3+\cdots}.$$

Thus, for example, we have

$$\sqrt{2} = \frac{2}{1+} \frac{1}{2+} \frac{1}{2+} \frac{1}{2+\cdots}.$$

If we have a continued fraction of the form

$$\frac{z}{a_1+} \frac{z}{a_2+} \frac{z}{a_3+\cdots},$$

then it is evident that the successive convergents are rational functions of z and in this section we will develop a method due to Thiele for determining a continued fraction approximation to a function.

First we recall Newton's divided difference interpolation formula

$$\begin{aligned} f(x) = & f(x_0) + (x - x_0)f[x_0, x_1] + (x - x_0)(x - x_1)f[x_0, x_1, x_2] + \cdots \\ & + (x - x_0)(x - x_1) \cdots (x - x_{n-1})f[x_0, x_1, \cdots, x_n] + R_n, \end{aligned} \quad (11.71)$$

where

$$R_n = (x - x_0)(x - x_1) \cdots (x - x_n)f[x_0, x_1, \cdots, x_n, x].$$

If $u_0(x) = f(x)$ and

$$u_r(x) = u_r(x_r) + (x - x_r)u_{r+1}(x),$$

then

$$u_r(x_r) = f[x_0, x_1, \dots, x_r],$$

the r th divided difference. Now let $v_0(x) = f(x)$ and define the sequence of functions $\{v_r(x)\}$ by

$$v_r(x) = v_r(x_r) + \frac{x - x_r}{v_{r+1}(x)} = b_r + \frac{x - x_r}{v_{r+1}(x)}. \quad (11.72)$$

Then

$$\begin{aligned} f(x) &= v_0(x), \\ &= v_0(x_0) + \frac{x - x_0}{v_1(x)}, \\ &= b_0 + \frac{x - x_0}{b_1 + \frac{x - x_1}{v_2(x)}}, \\ &= b_0 + \frac{x - x_0}{b_1 +} \frac{x - x_1}{b_2 + \frac{x - x_2}{v_3(x)}}, \\ &= \dots \\ &= b_0 + \frac{x - x_0}{b_1 +} \frac{x - x_1}{b_2 +} \dots \frac{x - x_{n-1}}{b_n +} \frac{x - x_n}{v_{n+1}(x)} \end{aligned} \quad (11.73)$$

In general it is not easy to obtain $v_{n+1}(x)$ but we note that when x takes the values x_0, x_1, \dots, x_n the value of $v_{n+1}(x)$ is not required and we obtain a terminating continued fraction which, at the points x_0, x_1, \dots, x_n agrees with $f(x)$.

To find the b_r we have from (11.72)

$$v_{r+1}(x) = \frac{x - x_r}{v_r(x) - v_r(x_r)},$$

so that, defining $\phi_0[x] = f(x)$, we generate a sequence of functions $\{\phi_r\}$ as follows

$$\begin{aligned} v_1(x) &= \frac{x - x_0}{v_0(x) - v_0(x_0)} = \frac{x - x_0}{f(x) - f(x_0)} = \phi_1[x_0, x], \\ v_2(x) &= \frac{x - x_1}{\phi_1[x_0, x] - \phi_1[x_0, x_1]} = \phi_2[x_0, x_1, x], \end{aligned}$$

and, in general,

$$v_r(x) = \frac{x - x_{r-1}}{\phi_{r-1}[x_0, \dots, x_{r-2}, x] - \phi_{r-1}[x_0, \dots, x_{r-1}]} = \phi_r[x_0, \dots, x_{r-1}, x]. \quad (11.74)$$

The functions ϕ_r , by analogy with divided differences, are called *inverted differences* and we note that

$$b_r = \phi_r[x_0, \dots, x_r], \quad (11.75)$$

so that we can easily build up our continued fraction. Inverted differences, unlike divided differences, are not symmetric functions of their argument. We can obtain symmetry by defining

$$\rho_r[x_0, \dots, x_r] = \phi_r[x_0, \dots, x_r] + \phi_{r-2}[x_0, \dots, x_{r-2}] + \phi_{r-4}[x_0, \dots, x_{r-4}] + \dots, \quad (11.76)$$

which terminates with $\phi_1[x_0, x_1]$ if r is odd and $\phi_0[x_0] = f(x_0)$ if r is even. $\rho_r[x_0, \dots, x_r]$ is called a *reciprocal difference* and is a symmetric function of the arguments.

In the Newton divided difference interpolation formula if all x_i tend to x_0 then we obtain the Taylor expansion of $f(x)$ about x_0 . A similar limiting process applies to the continued fraction representation and as $x_i \rightarrow x_0$ (all i), $b_r \rightarrow c_r$ (all r) so that

$$\begin{aligned} f(x) &= b_0 + \frac{x - x_0}{b_1 +} \frac{x - x_1}{b_2 + \dots} \frac{x - x_{n-1}}{b_n}, \\ &\rightarrow c_0 + \frac{x - x_0}{c_1 +} \frac{x - x_0}{c_2 + \dots} \frac{x - x_0}{c_n}. \end{aligned} \quad (11.77)$$

This expansion is called a Thiele expansion and we shall now explain how the c 's are obtained. Since

$$b_r = \phi_r[x_0, \dots, x_r] = \rho_r[x_0, \dots, x_r] - \rho_{r-2}[x_0, \dots, x_{r-2}],$$

we have, if we write

$$\begin{aligned} \phi_r(x) &= \lim_{x_i \rightarrow x} \phi_r[x_0, \dots, x_r], & i = 0, 1, \dots, r, \\ \rho_r(x) &= \lim_{x_i \rightarrow x} \rho_r[x_0, \dots, x_r], & i = 0, 1, \dots, r, \end{aligned}$$

and rearrange

$$\rho_r(x) = \rho_{r-2}(x) + \phi_r(x). \quad (11.78)$$

Substitution of $x_i = x$, $i = 0, 1, \dots, r-1$ in (11.74) gives

$$\begin{aligned} \phi_r[x, \dots, x, x_r] &= \frac{x_r - x}{\phi_{r-1}[x, \dots, x, x_r] - \phi_{r-1}[x, \dots, x, x]}, \\ &= \frac{x_r - x}{\rho_{r-1}[x, \dots, x, x_r] - \rho_{r-1}[x, \dots, x, x]}, \end{aligned}$$

and as $x_r \rightarrow x$ we have

$$\phi(x) = 1 / \frac{\partial}{\partial x} \rho_{r-1}[x, \dots, x].$$

In particular,

$$\phi_r(x) = r \left/ \frac{d\rho_{r-1}(x)}{dx} \right. . \quad (11.79)$$

(11.78) and (11.79) enable us to determine the quantities $c_r = \phi_r(x_0)$. The functions $\phi_r(x)$ are called the inverse derivatives of the function $f(x)$.

11.6 The method of Steepest Descent

This method can be a valuable tool for determining an asymptotic expansion for the inverse Laplace transform when t is large — this may of course not always be possible as is the case when $f(t) = \cos t$. Consider the integral

$$I = \int_{\mathcal{C}} h(z) e^{tg(z)} dz,$$

where t is a large positive parameter, $g(z)$ is an analytic function and \mathcal{C} , the path of integration is an arc or closed contour in the complex plane. This integral will be unchanged if \mathcal{C} is deformed provided that the path does not pass through a singularity of the integrand. If we write $z = x + iy$, $g(z) = u(x, y) + iv(x, y)$, the integrand becomes

$$h(x + iy) e^{itv} e^{tu}.$$

For constant v and large t the integrand does not oscillate rapidly and if $u(x, y)$ is large and positive the modulus of the integrand is also large for all v . At an extremum of u

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial y} = 0,$$

and, by virtue of the Cauchy-Riemann equations,

$$\frac{\partial v}{\partial x} = \frac{\partial v}{\partial y} = 0$$

at this extremum. Since we also have

$$\frac{\partial^2 u}{\partial x^2} = -\frac{\partial^2 u}{\partial y^2} \quad \text{and} \quad \frac{\partial^2 v}{\partial x^2} = -\frac{\partial^2 v}{\partial y^2},$$

it follows that if u is a maximum in the x direction it is a minimum in the y direction and vice versa. Such an extreme point is called a saddle point because the shape of the curve at the extremum is shaped like a horse's saddle. If z_0 is the saddle point then, from the above, it follows that $g'(z_0) = 0$ and in order to obtain a path of steepest descent from z_0 it is sufficient to select the contour by requiring that the term involving g'' in the expansion

$$g(z) = g(z_0) + \frac{1}{2}(z - z_0)^2 g''(z_0) + \dots,$$

be real and negative for $z \in \mathcal{C}$ and in the neighbourhood of z_0 . This gives

$$I \sim e^{tg(z_0)} \int_{\mathcal{C}} h(z) \exp\left[\frac{1}{2}(z - z_0)^2 g''(z_0)\right] dz,$$

or, substituting $s^2 = -t(z - z_0)^2 g''(z_0)$, we have

$$I \sim \frac{e^{tg(z_0)}}{[-tg''(z_0)]^{1/2}} \int_{-\infty}^{\infty} h(z) e^{-\frac{1}{2}s^2} ds. \quad (11.80)$$

The main contribution to the integral is obtained by putting $h(z) = h(z_0)$ which is equivalent to evaluating the integral in the neighbourhood of the saddle point.

Example 11.6 Find the asymptotic expansion of $f(t)$ for *small* t given that

$$\bar{f}(s) = s^{-1/2} e^{-2s^{1/2}}.$$

By the inversion formula

$$f(t) = \mathcal{L}^{-1}\{\bar{f}(s)\} = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} s^{-1/2} e^{ts-2s^{1/2}} ds, \quad \Re \gamma > 0.$$

Let $s = \sigma/t^2$. Then

$$f(t) = \frac{1}{2\pi i t} h(1/t),$$

where

$$h(\lambda) = \int_{\gamma-i\infty}^{\gamma+i\infty} \sigma^{-1/2} \exp(\lambda[\sigma - 2\sigma^{1/2}]) d\sigma, \quad \Re \gamma > 0.$$

We now analyze the asymptotic behaviour of the integral $h(\lambda)$ as $\lambda \rightarrow \infty$, i.e., as $t \rightarrow 0+$. We need to determine the saddle point which is the solution of

$$\frac{d}{d\sigma}[\sigma - 2\sigma^{1/2}] = 0,$$

that is $\sigma = 1$.

To evaluate the integral we set $\sigma = \rho e^{i\theta}$ noting that, because of the branch cut on the negative real axis, $\theta \in (-\pi, \pi)$. It follows that the steepest descent and ascent paths can be shown to be $\sqrt{\rho} \cos(\theta/2) - 1 = 0$ and $\theta = 0$. Thus, if we deform the path of integration to be the steepest descent path, we find that

$$h(\lambda) \sim 2i\sqrt{\pi}\lambda^{-1/2}e^{-\lambda} \quad \text{as } \lambda \rightarrow \infty.$$

Thus,

$$f(t) \sim \frac{e^{-1/t}}{\sqrt{\pi t}} \quad \text{as } t \rightarrow 0+.$$

This agrees with the tabulated transform given in Appendix 11.1.

11.7 Gerschgorin's theorems and the Companion Matrix

If $p(z)$ is a polynomial of degree n with leading term z^n , that is,

$$p(z) = z^n + a_1 z^{n-1} + a_2 z^{n-2} + \cdots + a_{n-1} z + a_n,$$

then the roots of the equation $p(z) = 0$ are exactly the eigenvalues of the companion matrix, C ,

$$C = \begin{bmatrix} -a_1 & -a_2 & -a_3 & \cdots & -a_{n-1} & -a_n \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

Gerschgorin's theorems give information about the location of the eigenvalues of a general matrix A (see Wilkinson [254]).

Theorem 11.1 *If $A = (a_{ij})$ is a $n \times n$ matrix then every eigenvalue λ of A lies in at least one of the circular discs with centres a_{ii} and radii $\sum_{j \neq i} |a_{ij}|$, that is, in the union of the discs*

$$|\lambda - a_{ii}| \leq \sum_{j(\neq i)} |a_{ij}|, \quad i = 1, \dots, n.$$

■

Theorem 11.2 *If s of the circular discs of Theorem 11.1 form a connected domain which is isolated from the other discs, then there are precisely s eigenvalues of A within this connected domain.*

■

It follows from Theorem 11.1 that the eigenvalues of the companion matrix C lie in the union of the discs

$$\begin{aligned} |-a_1 - z| &\leq 1, \\ |z| &\leq |a_j| + 1, \\ |z| &\leq |a_n|, \end{aligned}$$

and consequently that the roots of the polynomial equation $p(z) = 0$ satisfy

$$|z| \leq \max_j (|a_j| + 1), \quad j = 1, \dots, n.$$

With regard to the polynomial in Application 10.1 the companion matrix has

$$a_1 = -\left(1 + \frac{\mu + s}{\lambda}\right), \quad a_2 = \cdots = a_{N-1} = 0, \quad a_N = \mu/\lambda,$$

and its eigenvalues lie in the union of the discs

$$|z| \leq 1, \quad |z| \leq \mu/\lambda,$$

and

$$\left| z + 1 + \frac{\mu + s}{\lambda} \right| \leq 1.$$

If $\mu \leq \lambda$ then N of the discs are unit discs and the remaining disc is isolated from the unit discs if $|(\mu + s)/\lambda| > 1$, i.e., if s satisfies $|s| > \lambda - \mu$ (which implies $\Re s > \gamma$ for some γ).

Another application of Gerschgorin's theorems arises in Weeks's method where, in choosing the parameters of the method, we need bounds for the zeros of the Laguerre polynomials. In Cohen [45] it is noted that the zeros of the Laguerre polynomial $L_n(x)$ are the eigenvalues of the symmetric tridiagonal matrix

$$A = \begin{bmatrix} 1 & 1 & & & & & \\ 1 & 3 & 2 & & & & \\ & 2 & 5 & 3 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & n-2 & 2n-3 & n-1 & \\ & & & & n-1 & 2n-1 & \end{bmatrix}. \quad (11.81)$$

Application of Gerschgorin's theorem shows that the largest root of the equation $L_n(x) = 0$ satisfies

$$\lambda \leq \max(4n - 6, 3n - 2),$$

i.e.,

$$\lambda \leq 4n - 6, \quad n \geq 4.$$

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