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Methods of Numerical Integration for Rapidly Oscillatory Integrals

by

Jonathan Robert Webster

A Doctoral Thesis
submitted in partial fulfilment of the requirements for the award of
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October, 1999

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Abstract

This thesis is concerned with the evaluation of rapidly oscillatory integrals, that is integrals in which the integrand has numerous local maxima and minima over the range of integration. Three numerical integration rules are presented. The first is suitable for computing rapidly oscillatory integrals with trigonometric oscillations of the form $f(x) \exp(i\pi q(x))$. The method is demonstrated, empirically, to be convergent and numerically stable as the order of the formula is increased. For other forms of oscillatory behaviour, a second approach based on Lagrange's identity is presented. The technique is suitable for any oscillatory weight function, provided that it satisfies an ordinary linear differential equation of order $m \geq 1$. The method is shown to encompass Bessel oscillations, trigonometric oscillations and Fresnel oscillations, and products of these terms. Examples are included which illustrate the efficiency of the method in practical applications. Finally, integrals where the integrand is singular and oscillatory are considered. An extended Clenshaw-Curtis formula is developed for Fourier integrals which exhibit algebraic and logarithmic singularities. An efficient algorithm is presented for the practical implementation of the method.
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Chapter 1

Introduction

1.1 Introduction

Many problems in applied mathematics give rise to rapidly oscillatory integrals, that is integrals in which the integrand has numerous local maxima and minima over the range of integration. The principal examples of such integrals occur in the solution of ordinary and partial differential equations, in the form of integral transforms. Particular instances include the Fourier transform

\[ \int_a^b e^{ixf(x)} \, dx, \]

and the Fourier-Bessel transform

\[ \int_0^1 J_n(\gamma_m x)f(x) \, dx, \]

where \( 0 < \gamma_1 < \gamma_2 < \cdots \) are the zeros of the Bessel function \( J_n(x) \). Many other examples of highly oscillatory integrals may be found in recent research into coherent optical imaging [58], the study of water waves on a sloping beach [15] and the analysis of spin in quantum mechanics [64].

The numerical evaluation of such rapidly oscillatory integrals is a particularly difficult problem. Few oscillatory integrals that arise in practice can be

\[^{1}\text{Davis and Rabinowitz [12] define numerous to be "more than 10".}\]
evaluated using analytic mathematical techniques. Furthermore, standard methods of approximate integration typically prove inadequate. For example, consider the diffraction integral

\[ C(x, y, \beta) = \frac{1}{2\beta} \int_{-\beta}^{\beta} \cos(x \cos \theta - y \sin \theta) \cos \theta \, d\theta, \]

as analysed by Hartree [36]. One way to evaluate this integral is to apply the method implicit in the fundamental theorem of the calculus, that is find a primitive function \( F(\theta) \) such that

\[ F'(\theta) = \cos(x \cos \theta - y \sin \theta) \cos \theta. \]

Then

\[
C(x, y, \beta) = \frac{1}{2\beta} \int_{-\beta}^{\beta} \cos(x \cos \theta - y \sin \theta) \cos \theta \, d\theta = \frac{1}{2\beta} \int_{-\beta}^{\beta} F'(\theta) \, d\theta = \frac{1}{2\beta} [F(\beta) - F(-\beta)].
\]

The difficulty with this approach lies in obtaining a suitable expression for the primitive function. In this particular instance, \( F(\theta) \) cannot be expressed in finite terms by a combination of algebraic, logarithmic and exponential functions and other representations, in the form of infinite series for example, are not suited to numerical computation.

An alternative approach is to evaluate \( C(x, y, \beta) \) using an approximate integration formula, for example the Gauss-Legendre [21, pp. 40-51] or Clenshaw-Curtis [10] formulas. In each case the integrand is approximated using polynomials, which for small values of \( x \) and \( y \) is a successful strategy. However, as \( x \) and \( y \) increase in magnitude, the integrand looks less and less like a polynomial of any given degree and the integration formulas prove correspondingly less effective.

These types of problem are typical. The standard mathematical techniques, such as contour integration or the fundamental theorem, rarely work on real-world examples. Even if they do work, their application may be sufficiently complicated
for one to pause before continuing. Similarly, conventional methods of numerical integration are ill-suited to the evaluation of rapidly oscillatory integrals. Nearly all approximate the entire integrand using a polynomial approximation, which is obviously a poor choice when dealing with oscillatory functions.

To overcome these difficulties, a number of numerical integration schemes have been developed specifically for the evaluation of highly oscillatory integrals. In many instances, the methods have been proposed by researchers whose work into other areas of mathematics has led them to a particular type of integral. Others have been developed simply to fill a gap in the existing technology. Whatever the motivation, there is now a wide range of numerical methods that may be used to evaluate rapidly oscillatory integrals. In the next two sections we discuss some of the most commonly applied methods. Section 1.2 deals with schemes specific to integrals over a finite range, while the infinite and semi-infinite cases are covered in Section 1.3.

1.2 Finite range oscillatory integrals

Numerical methods for evaluating oscillatory integrals over a finite range are usually developed with a specific oscillatory kernel in mind. In many instances, however, the principles on which the formulas are based are identical, regardless of the oscillatory term, and this allows them to be studied within a common framework. With this in mind the contents of this section are organised on the following basis. First, where appropriate, we give a brief overview of the ideas behind a particular type of integration formula, and then we consider some specific implementations.

1.2.1 Product integration rules

Product integration rules [12, pp. 74-92] are probably the most widely used numerical method for dealing with integrals where the integrand contains an "awkward" factor, such as a singular or oscillatory term. The idea behind product integration
is to split the integrand into the product of two terms, the first a weight function \( w(x) \) that represents the troublesome factor, and the other a smooth function \( f(x) \). The integral is then approximated using the formula

\[
\int_a^b w(x)f(x) \, dx \approx \sum_{j=0}^n w_j f(x_j),
\]

where the integration weights are chosen to make the rule exact if \( f(x) \) is any polynomial of degree \( \leq n \). The weight function \( w(x) \) does not appear explicitly in the integration formula and so is used to eliminate the awkward term. The abscissae \( x_0, \ldots, x_n \) are all assumed to be fixed and distinct numbers lying between \( a \) and \( b \).

The most common way to generate formula (1.2.1) is to approximate \( f(x) \) using the polynomial \( p_n(f; x) \) \cite[pp. 131-138]{6} that interpolates it at the points \( x_0, \ldots, x_n \). The interpolating polynomial can then be integrated and the result expressed in the form given above. An alternative approach is to make the error in the integration rule

\[
E(f) = \int_a^b w(x)f(x) \, dx - \sum_{j=0}^n w_j f(x_j)
\]

zero for the functions 1, \( x, x^2, \ldots, x^n \). This gives a system of linear algebraic equations for the integration weights, which has a unique solution as all the abscissae are distinct.

In both cases, the computation of the integration weights depends upon being able to evaluate a set of auxiliary integrals. If the first method is used and the interpolating polynomial has the form

\[
p_n(f; x) = \sum_{k=0}^n d_k q_k(x),
\]

where \( \{q_k(x)\} \) is some convenient set of polynomials, then the integrals

\[
\int_a^b w(x)q_k(x) \, dx, \quad k = 0, 1, \ldots, n
\]

are required explicitly. If the second method is used, the integrals

\[
\int_a^b w(x)x^k \, dx, \quad k = 0, 1, \ldots, n
\]
are needed in place of (1.2.4).

In practice, the evaluation of the auxiliary integrals is usually extremely difficult. In most instances simple closed form expressions are not available and the integrals have to be evaluated using special numerical techniques. A rule of thumb in these cases, is that computing (1.2.4) or (1.2.5) should be at least an order of magnitude easier than computing the original integral, otherwise there is little or no benefit to be found in generating a product integration rule.

From the point of view of oscillatory integrals, a number of successful attempts have been made to implement product integration rules, but only for the particular weight functions $w(x) = e^{itx}$ and $w(x) = J_v(tx)$. The reason for this, is that in these two instances, the auxiliary integrals are relatively straightforward to evaluate, whereas for other oscillatory kernels this typically isn't the case.

For trigonometric integrals, the product integration rules fall into two main categories: those which are oscillatory equivalents of the Newton-Cotes rules [21, pp. 35-40] and depend on approximating $f(x)$ by a low order interpolating polynomial based on equal spaced points, and those which are equivalent to the Clenshaw-Curtis formula [10], where the approximation is with Chebyshev polynomials using cosine-distributed points.

In the first case, the integration formulas are straightforward to generate, as the auxiliary integrals are available in closed form. A particular example of this type of formula is Filon's [29] method, in which $f(x)$ is approximated by a quadratic polynomial to give an oscillatory version of Simpson's rule. Other approaches in a similar vein include Tuck [79], who produces a trapezoidal equivalent, Clendenin [9] and Luke [47] who uses polynomials of degree $\leq 10$. A further extension is given by Alaylioglu, Evans and Hyslop [4], who implement a recursive routine for computing the general formula.

In the second case the situation is slightly more complicated, as the auxiliary integrals

$$\int_{-1}^{1} e^{irx} T_k(x) dx, \quad k = 0, 1, \ldots, n, \quad (1.2.6)$$
have no apparent closed form and so must be computed numerically. Piessens and Poleunis [62] suggest expanding the integrals as Neumann series, but this approach is computationally expensive for large $\tau$. More effective alternatives include the use of recurrence relations, Patterson [57], Sloan and Smith [72], expanding the integrals as a series of spherical Bessel functions, Littlewood and Zakian [44], and obtaining expressions in terms of hypergeometric functions, Adam and Nobile [2]. A comparison of these methods is presented in Evans and Webster [28].

For Bessel function integrals the situation is very similar. Piessens and Branders [61] have developed an extended Clenshaw-Curtis method in which $f(x)$ is approximated using a finite Chebyshev expansion. The auxiliary integrals

$$\int_{-1}^{1} J_\nu(\tau \hat{x}) T_k(x) dx, \quad \hat{x} = Ax + B, \quad (1.2.7)$$

are then computed using an eight-term recurrence relation. Evans [20] presents a similar method, but avoids the direct computation of the integrals (1.2.7) by expanding the Chebyshev polynomials as powers of $x$, a method also used in the trigonometric case [5].

1.2.2 Use of approximations

Product integration rules are a subset of a wider class of numerical integration formulas based on approximations. The basic principle is to find a sequence of functions $f_0(x), f_1(x), \ldots$ that approximate $f(x)$ over the interval of integration, each of which can be integrated more easily than $f(x)$ itself. The integral of the approximation then constitutes an approximation to the original integral.

A common form for the approximation is a series expansion

$$f_n(x) = \sum_{k=0}^{n} a_k \phi_k(x), \quad a \leq x \leq b, \quad (1.2.8)$$

in which the basis functions $\phi_k(x)$ are chosen to give an accurate fit to $f(x)$ over the interval $[a, b]$. In this case, the approximation to the original integral can be
expressed as
\[ \int_a^b w(x)f(x)\,dx \approx \sum_{k=0}^n a_k M_k, \tag{1.2.9} \]
where
\[ M_k = \int_a^b w(x)\phi_k(x)\,dx, \quad k = 0, 1, \ldots, n. \tag{1.2.10} \]
As with product integration rules, the auxiliary integrals (1.2.10) should be easier to evaluate than the original integral.

In the case where the coefficients \( a_k \) are determined by interpolating \( f(x) \) at \( n + 1 \) distinct points \( x_0, x_1, \ldots, x_n \) in the interval \( [a, b] \), a formula equivalent to (1.2.9) may be generated by making the approximate integration rule
\[ \int_a^b w(x)f(x)\,dx \approx \sum_{j=0}^n w_j f(x_j) \tag{1.2.11} \]
exact for the functions \( f = \phi_0(x), \ldots, \phi_n(x) \). For the particular choice \( \phi_k = x^k \) this formula reduces to the product integration rule of the previous section.

Particular examples of this approach for the integral
\[ \int_a^b e^{ir\tau(x)} f(x)\,dx \tag{1.2.12} \]
are considered by Ehrenmark [16] and Evans [24]. Ehrenmark constructs a three-point formula that is exact for the functions 1, \( \sin kx \), \( \cos kx \) and employs the mid-point and two end-points of the interval \( [a, b] \). Integrals of the form (1.2.12) are handled by applying the formula with \( k \) taken to be the average of \( \tau q'(x) \) over \( [a, b] \). Evans takes a different approach and approximates \( f(x) \) in the form
\[ f(x) \approx q'(x) \sum_{k=0}^n a_k g_k(q(x)), \tag{1.2.13} \]
where the functions \( g_k(q) \) are chosen to give an accurate fit over \( [a, b] \). The auxiliary integrals corresponding to (1.2.10) are computed either analytically or numerically depending on the form of \( g_k(q) \).

For the simpler Fourier integral \( \int e^{ir\tau(x)} f(x)\,dx \), integration formulas based on spline approximations are discussed by Dierckx and Piessens [13], Marti [53] and Neuman [55].
1.2.3 Integration between the local maxima

The idea behind this method is very simple: the local maxima (or minima) of the oscillatory part of the integrand are located, \( a \leq x_1 < x_2 < \ldots < x_p \leq b \), and each subintegral

\[
\int_{x_j}^{x_{j+1}} w(x)f(x) \, dx
\]  

(1.2.14)

is evaluated using a standard numerical integration rule, such as the Gauss-Legendre or Clenshaw-Curtis formulas. The approximation to the original integral is then given by summing the contributions from the individual subintegrals.

The advantages of this method are its simplicity and the fact that it may be applied to any form of oscillatory integral. The main disadvantage, is that it requires the local maxima (or minima) of the oscillatory part of the integrand. In some cases, such as \( w(x) = \sin \pi x \), these are easy to obtain analytically. However, for most oscillatory kernels this is not the case and the local maxima will have to be computed numerically. In such instances, the benefit of reducing the oscillatory integral to a series of non-oscillatory integrals has to be balanced against the additional effort required to compute the turning points.

For trigonometric integrals a simpler approach is to integrate between the zeros. In this case, it is a good idea to evaluate the subintegrals using a formula that employs the values of the integrand at the end-points of the interval of integration. Since the integrand is zero at these points additional accuracy is obtained without extra computation.

Developments of this method for trigonometric integrals are given by Price [63] and van de Vooren and van Linde [81]. A further extension, using a variation of the Euler transformation to speed up the convergence of the series of subintegrals, is considered by Longman [46].
1.2.4 Fourier integrals

In the particular case of the Fourier integral

\[ \int_a^b e^{i\tau x} f(x) \, dx, \]  

(1.2.15)
a number of other numerical integration schemes have been suggested. For example, Stetter [78] considers the asymptotic expansion of (1.2.15) in the form

\[ \int_a^b e^{i\tau x} f(x) \, dx \sim e^{i\tau b} \sum_{k=0}^{n} i^{k-1} f^{(k)}(b) \tau^{-k-1} - e^{i\tau a} \sum_{k=0}^{n} i^{k-1} f^{(k)}(a) \tau^{-k-1}, \]  

(1.2.16)
and uses this to construct a polynomial approximation of the integral in powers of \( 1/\tau \). Goldberg and Varga [31] present an alternative method based on Möbius inversion of the Poisson summation formula (MIPS) and this has been developed further in a series of articles by Lyness [48, 50, 51]. The use of Gaussian integration formulas has also been considered by Piessens [59, 60] and Gautschi [30].

1.3 Infinite range oscillatory integrals

The evaluation of oscillatory integrals over an infinite range is handled quite differently to the case of finite range integrals. The principle tool is the use of extrapolation techniques, where the essential idea is to split the integral into an infinite series of subintegrals and then accelerate the convergence of the partial sums of the series using a sequence transformation. In certain instances, where the asymptotic behaviour of the integrand is known, more effective extrapolation methods can be employed. Numerical integration schemes based on direct approximation of the integrand are less common than in the finite case, although a number have been developed to evaluate Fourier integrals.

1.3.1 Extrapolation techniques

The most commonly used extrapolation technique is a modification of integration between the zeros. The idea is to subdivide the integral into an infinite series of
subintegrals and use a sequence transformation to speed up the convergence of the partial sums of the series. A particular example of this technique is considered by Longman [45], who uses the Euler transformation [12, pp. 230-231] to accelerate the convergence. An alternative is to use the more effective transformation of Shanks [65], an approach suggested by Alaylioglu, Evans and Hyslop [3]. A similar method has also been proposed by Squire [76, 77], who considers the use of Aitken extrapolation and Levin's u- and v-transforms [40].

In the case where the asymptotic behaviour of the integrand is known, Sidi [67] has developed the W-transformation, which is an effective extrapolation method for evaluating a general class of oscillatory integrals. Sidi [69] has also developed a user friendly version of the W-transformation, which avoids the need for excessive asymptotic analysis of the integrand. A further extension, appropriate for infinite range oscillatory integrals defined in the sense of Abel summability, is given in Sidi [68].

An alternative extrapolation technique is the D-transformation of Levin and Sidi [43], which may be used to evaluate infinite range integrals provided the integrand satisfies a known linear differential equation. The D-transformation and two modifications are used by Sidi [66] specifically to evaluate oscillatory integrals over an infinite interval. A further transformation that has been used successfully to evaluate infinite range oscillatory integrals is the G-transformation of Gray, Atchison and McWilliams [34], which is a continuous equivalent of Shanks' transformation. Higher order G-transformations, which are more efficient than the original technique, are considered by Gray and Atchison [33].

1.3.2 Truncation of the infinite interval

An alternative way to evaluate oscillatory integrals over an infinite range is to reduce the infinite interval to a finite range by ignoring the tail of the integrand. The successful application of this technique requires an efficient method to evaluate the finite range integral and some way of estimating the discarded tail. In
practice, this usually limits the use of the method to trigonometric and Bessel integrals.

Two examples of this approach for the Fourier integral

\[ \int_{0}^{\infty} e^{ix\tau} f(x) \, dx \]  

are given by Pantis [56] and Gustafson and Dahlquist [35]. Pantis uses Filon's method to compute the finite range integral and estimates the tail using the asymptotic expansion

\[ -e^{-ir\tau} \int_{k}^{\infty} e^{i\tau x} f(x) \, dx \sim \frac{f(k)}{i\tau} - \frac{f'(k)}{(i\tau)^2} + \cdots. \]  

Gustafson and Dahlquist take a different approach and approximate \( f(x) \) over the range \( [k, \infty] \) by exponential sums, to give an approximation of the tail as a rational function of \( \tau \).

1.3.3 Fourier integrals

As in the finite range case, a number of additional methods have been developed specifically for the evaluation of Fourier integrals. Probably the most important technique is the use of the Fast Fourier Transform [12, pp. 246-264] to efficiently compute Discrete Fourier Transform approximations of the Fourier integral. Alternative methods, based on approximating the non-oscillatory part of the integrand, have also been suggested. For example, Krylov and Skoblya [39] consider the Fourier cosine integral

\[ \int_{0}^{\infty} \cos \tau x f(x) \, dx, \]  

and linearly interpolate \( f(x) \) at the points \( 0, h, 2h, \ldots \), and integrate over each subinterval to obtain the approximation

\[ \int_{0}^{\infty} \cos \tau x f(x) \, dx \approx \frac{2 - 2 \cos \tau h}{\tau^2 h} \sum_{k=0}^{\infty} \cos k\tau h f(kh), \]  

with a similar formula for the Fourier sine integral. Silliman [70] has generalised this approach by using spline functions to approximate \( f(x) \). Another method,
relevant for the Fourier integrals
\[ \int_0^\infty x^\alpha e^{-x} e^{ix^2} f(x) \, dx, \quad (1.3.5) \]
and
\[ \int_{-\infty}^\infty e^{-x^2} e^{ix^2} f(x) \, dx, \quad (1.3.6) \]
has been proposed by Patterson [57]. The idea is to approximate \( f(x) \) using Laguerre or Hermite expansions respectively, in which case the closed form expressions
\[ \frac{k!}{\Gamma(k+1+\alpha)} \int_0^\infty x^\alpha e^{-x} e^{ix} L_k^{(\alpha)}(x) \, dx = i^{1+\alpha} \tau^k \left( \frac{\tau - i}{1 + \tau^2} \right)^{k+1+\alpha}, \quad (1.3.7) \]
and
\[ \int_{-\infty}^\infty e^{-x^2} e^{ix} H_k(x) \, dx = i^k \pi^{1/2} \tau^k e^{-\tau^2/4}, \quad (1.3.8) \]
may be used to complete the integration.

1.4 Summary

The numerical schemes just presented should not disguise the fact that difficult integrals requiring special study and treatment still occur frequently in applications. Particularly tough integrals are finite range integrals in which the oscillatory kernel is something other than a regular trigonometric function or a single Bessel function. A prime example would be
\[ \int_a^b C(q(x)) f(x) \, dx, \quad -\infty < a < b < \infty, \]
where \( C(x) \) is the Fresnel Cosine integral [1, pp. 295-331]. In this case, the methods outlined in Section 1.2 have no obvious counterparts. Another important class of integrals that are very difficult to evaluate are those involving products of Bessel functions,
\[ \int_a^b J_\nu(q_1(x)) J_\mu(q_2(x)) f(x) \, dx, \]
and combinations of trigonometric and Bessel functions,

\[ \int_a^b e^{i\varphi_1(x)} J_\nu(q_2(x)) f(x) \, dx. \]

Integrals of this type are increasingly common in applications, but the difficult nature of the problem has meant that very few numerical methods have been proposed for their evaluation.

The aim of this thesis is to introduce new methods of numerical integration that address the evaluation of these types of integral. In Chapter 2 we develop an effective integration scheme for the evaluation of irregular trigonometric integrals. In Chapter 3 this method is extended to a general class of oscillatory integrals, which includes Bessel product integrals and Bessel-trigonometric integrals as particular cases. The evaluation of integrals where the integrand is singular and oscillatory is considered in Chapter 4. Conclusions and recommendations for further research are given in Chapter 5.

In the course of preparing this thesis, five papers have been published in refereed journals and one conference paper has been presented. The details may be found in references [8, 26, 27, 28, 83] and [82] respectively.
Chapter 2

A method to evaluate irregular trigonometric integrals

2.1 Introduction

Many problems in physics and applied mathematics give rise to irregular trigonometric integrals, that is integrals of the form

$$I(j, q, r) = \int_a^b e^{i\tau q(x)} f(x) \, dx, \quad -\infty < a \leq x \leq b < \infty,$$

(2.1.1)

where $f(x)$ is non-oscillatory and $|\tau q'(x)| \gg (b - a)^{-1}$. Traditionally, these have been evaluated using asymptotic techniques, such as stationary phase or steepest descent expansions. However, motivated by the occurrence of such integrals in many problems currently being investigated, a number of alternative methods for their direct evaluation have recently been proposed. The purpose of this chapter is to discuss these methods and compare their effectiveness against a newly developed integration scheme.

2.2 The existing methods

Integrals of the form (2.1.1) arise throughout physics and applied mathematics, in fields as diverse as coherent optical imaging [58], the study of water waves...
on a sloping beach [15], and in the analysis of spin in quantum mechanics [64].

The traditional way to evaluate these integrals is to use asymptotic methods,
such as steepest descent or stationary phase expansions [18], but in general these
techniques only deliver low accuracy. In most instances, their application requires
a considerable amount of analysis and it is often difficult to obtain anything other
than first order approximations. As a consequence of this, recent research has
focussed on developing numerical methods which can accurately evaluate (2.1.1)
and which involve a minimal amount of analysis of the integral.

An ideal way to do this, is to construct a product integration rule in the
Newton-Cotes or Clenshaw-Curtis style. The problem with this approach, is that
almost any attempt to approximate \( f(x) \) by powers of \( x \) or Chebyshev polynomials
results in a series of integrals which are as difficult to evaluate as the original
integral. One way to overcome this difficulty, suggested by Evans [24], is to
approximate \( f(x) \) in the form

\[
f(x) \approx q'(x) \sum_{k=0}^{n} a_k g_k(q(x))
\]  

(2.2.1)

for some suitable choice of functions \( g_k(q) \). This reduces the original integral to a
series of Fourier integrals

\[
\int_{q(a)}^{q(b)} e^{i r q} g_k(q) \, dq, \quad k = 0, 1, \ldots, n,
\]  

(2.2.2)

which may be evaluated either analytically if \( g_k(q) = q^k \) or numerically using the
extended Clenshaw-Curtis method described in [28] for more general \( g_k(q) \). The
approximation itself is carried out by collocating \( f(x) \) with the series (2.2.1) at a
set of \( n + 1 \) distinct points in the interval \([a, b]\), giving a system of linear algebraic
equations for the coefficients \( a_k \).

An alternative method has been proposed by Levin [41], who notes that if
\( f(x) \) has the form

\[
f(x) = i r q'(x)p(x) + p'(x)
\]  

(2.2.3)

then the integral (2.1.1) integrates exactly to give

\[
I(f, q, \tau) = e^{i r q} p(x)|_a^b.
\]  

(2.2.4)
CHAPTER 2. IRREGULAR TRIGONOMETRIC INTEGRALS

Equation (2.2.3) is treated as an ordinary differential equation for \( p(x) \) despite there being no boundary condition to use. This omission is overcome by first proving that if \( f(x) \) and \( q'(x) \) are slowly oscillatory then there exists a slowly oscillatory solution of (2.2.3), which may be highlighted by the basis set method for ordinary differential equations. Specifically the form

\[
p(x) = \sum_{k=0}^{n} a_k u_k(x)
\]  

(2.2.5)

is tried with \( u_k(x) \) slowly oscillatory, typically \( u_k(x) = x^k \), and with collocation at points spaced equally across the interval. The coefficients \( a_k \) are determined by solving the resulting system of complex linear equations.

An obvious, but somewhat overlooked, method has been considered by Evans [22]. The idea is to use the transformation \( y = q(x) \) to convert (2.1.1) into the conventional Fourier integral

\[
\int_{q(a)}^{q(b)} f(q^{-1}(y)) e^{ir \gamma} dy,
\]

(2.2.6)

which may again be evaluated using the extended Clenshaw-Curtis method. This approach proves particularly straightforward if \( q(x) \) is simple enough to allow the inverse function to be obtained analytically, otherwise a robust numerical method must be used to compute the inverse.

Two simple approaches that avoid the use of \( q'(x) \) are described in Evans [23]. In the first method, \( f(x) \) and \( q(x) \) are approximated by linear functions, to give the irregular oscillatory equivalent of the trapezoidal rule. Hence, if the interval \([a, b]\) is subdivided into \( n \) equal subintervals, the integration rule may be written as

\[
\int_{a}^{b} e^{irq(x)} f(x) dx \approx \sum_{j=1}^{n} \int_{a+ (j-1) h}^{a+ j h} e^{ir(\alpha_j x + \beta_j)} (r_j x + s_j) dx,
\]

(2.2.7)

where \( h = (b - a)/n \). The second method is similar but uses quadratic approximations over each subinterval to give a formula equivalent to Simpson's rule. The implementation is straightforward in the linear case as the integrals on the r.h.s of (2.2.7) are available in closed form. However, in the second case the auxiliary
integrals
\[ \int_{a+(j-1)h}^{a+jh} e^{i(\alpha_j x^2 + \beta_j x + \gamma_j)} (\tau_j x^2 + s_j x + t_j) \, dx \]  
(2.2.8)
cannot be evaluated analytically and representations in terms of Fresnel integrals [1, pp. 295-331] are required to achieve a fast implementation.

One further method, proposed by Ehrenmark [16], is to construct a three point integration rule
\[ \int_a^b g(x) \approx \sum_{j=1}^3 w_j g(x_j) \]  
(2.2.9)
which is exact for the functions 1, \( \sin kx \), \( \cos kx \) using the mid-point and two end-points of the interval \([a, b]\). This gives a set of three linear algebraic equations that are used to determine the integration weights, \( w_1, w_2 \) and \( w_3 \). Integrals of the form (2.1.1) are then handled by applying the formula with \( k \) taken to be the average of \( \tau q'(x) \) over the interval \([a, b]\). In fact the results are fairly insensitive to the choice of \( k \), and the use of the maximum frequency in the interval may be employed as an alternative strategy.

When confronted with an integral of the form (2.1.1) the choice of method is not always entirely straightforward and may be influenced by a number of factors. For example, if \( q(x) \) is computed numerically, the only available options are the linear and quadratic rules of Evans, or Ehrenmark's three point formula, as the others require an explicit expression for \( q'(x) \). However, each of these methods uses low order approximations of \( f(x) \) and \( q(x) \), and as a consequence high levels of subdivision are needed to produce accurate results. They also have the added disadvantage of requiring increased levels of subdivision as \( \tau \) increases, a consequence of the way they sample \( q(x) \). For Ehrenmark's formula the number of function evaluations rises linearly with \( \tau \), and for the linear or trapezoidal formula as \( \sqrt{\tau} \). The quadratic rule is less affected and exhibits a cube-root dependence on \( \tau \).

If \( q'(x) \) is available, as is often the case (and which incidentally would be required to obtain either steepest descent or stationary phase approximations), then an improvement in efficiency may be obtained by using the three remaining
methods, although even here difficulties may still arise. For instance, if \( q'(x) \) has zeros in the interval \([a, b]\), then the transformation \( y = q(x) \) cannot be applied directly as the inverse function will be multivalued. One way around this is to locate the zeros of \( q'(x) \) and split the original integral into a series of integrals between these points. The method may then be applied to each of these in turn. Unfortunately, this approach leads to a set of integrals of the form (2.2.6) in which the non-oscillatory term is singular, a type of integral for which the extended Clenshaw-Curtis method is not well suited.

In the case of the expansion (2.2.1), some care has to be taken when choosing the functions \( g_k(q) \) to ensure that an accurate fit of \( f(x) \) is achieved. If this is not taken into consideration, the effectiveness of the method can suffer dramatically. For example, if \( q(x) = \cos x \), then the choice \( g_k = q^k \) behaves like powers of unity for small values of \( x \) and will not yield a collocating expansion in intervals around the origin. A further difficulty is that the linear equations used to obtain the coefficients \( a_k \) become ill-conditioned as \( n \) increases, and in practice use of the formula is limited to \( n \leq 16 \).

Similar problems arise with Levin’s method. Levin stresses the fact that the choice of basis functions \( u_k(x) \) will depend upon the form of \( f(x) \), and so it often necessary to analyse the solutions of (2.2.3) in order to choose an appropriate set. An example from Levin’s paper illustrates this point. The integral

\[
\int_0^{2\pi} \ln x \sin \tau x \, dx
\]  

is considered, with the associated differential equation

\[
irp(x) + p'(x) = \ln x.
\]

Near \( x = 0 \) the solution of (2.2.11) may be written as

\[
p(x) = \sum_{k=0}^{\infty} a_k x^k + \ln x \sum_{k=0}^{\infty} b_k x^k,
\]

which leads to the choice of functions

\[
u_k(x) = \begin{cases} 
x^{k-1} & \text{k odd,} 
x^{\frac{k}{2}} \ln x & \text{k even.}
\end{cases}
\]
Obviously, the need to indulge in such analysis gives an overhead that is difficult to quantify when comparing the different approaches, and it may mean that the method is abandoned in favour of a less accurate, but simpler rule, for example Ehrenmark's three point formula. Levin also indicates that difficulties arise with ill-conditioning in the linear equations for the coefficients $a_k$ and this limits the use of the formula to relatively low values of $n$. As a consequence, the only way to increase accuracy is to use repeated subdivision of the interval, a strategy that is often less efficient than the direct application of a high order formula.

With the above in mind, there is certainly scope for a method that retains or improves upon the accuracy of Levin's method or the formulas of Evans [22, 24], but eliminates, as much as is possible, the need to indulge in analytical aspects of mathematics.

In the next section, a variation on Levin's method is presented which addresses these points. The principle is to construct an integration rule that is exact for a choice of functions $P_k(x)$. Obviously, if the basis set used by Levin is identical to the choice of exact functions in the proposed method, and equal spaced points are used for the abscissae, then the same formula results. However, careful consideration of the choice of exact functions and, more importantly, the integration abscissae, has resulted in a version which allows the generation of high order formulas, with an associated improvement in accuracy. As a by product of this approach, a number of other advantages arise. For example, in contrast to Levin's method, in which $p(x)$ depends upon the values of $f(x)$ and requires recomputation for different functions, the proposed method generates a set of integration weights which may be used for any function. The method is also exact for a set of functions that are independent of $f(x)$ and $q(x)$, and this alleviates the need to determine specific basis functions for each problem. Another important benefit is that the method may be extended to handle other forms of oscillatory integral. This point is considered in depth in Chapter 3.

In the next section the integration rule itself is discussed. Given the motiva-
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...tion behind the recommended implementation, it is unlikely it would have arisen by considering Levin’s original philosophy. An example that illustrates the effectiveness of the new method is presented in Section 2.4. The results of numerical tests are reported in Section 2.5.

2.3 A new integration formula

To develop the integration rule for the integral (2.1.1), we first consider the particular case \( q(x) = x \), with a view to using the observations from this specific example as motivation for more general functions. Without loss of generality the interval \([a, b]\) is taken to be \([-1, 1]\). The idea is to approximate the integral using the formula

\[
\int_{-1}^{1} e^{i\pi x} f(x) \, dx \approx \sum_{j=0}^{n} w_j f(x_j),
\]

where the integration weights are chosen to make the rule exact for a set of functions \( f_k(x) \). If the functions are taken to be \( k = 0, 1, \ldots, n \),

\[
\sum_{j=0}^{n} w_j [i\pi p_k(x_j) + p'_k(x_j)] = [e^{i\pi x} p_k(x)]_{-1}^{1}, \quad k = 0, 1, \ldots, n
\]

immediately arise for the integration weights \( w_j \). Equation (2.3.2) is, of course, Levin’s differential equation and is used specifically to allow the auxiliary integrals

\[
\int_{-1}^{1} e^{i\pi x} f_k(x) \, dx, \quad k = 0, 1, \ldots, n
\]

to be evaluated easily in closed form.

With this formulation there is freedom in both the choice of functions \( p_k(x) \) and the abscissae \( x_j \). An obvious choice is to fix the abscissae as equal spaced

\[
x_j = -1 + 2j/n, \quad j = 0, 1, \ldots, n,
\]
with the functions $p_k(x)$ taken as
\[ p_k(x) = x^k, \quad k = 0, 1, \ldots, n. \quad (2.3.6) \]
This follows the spirit of the Newton-Cotes rules, and is the choice of collocation points used by Levin. Alternatively, an approach akin to the Clenshaw-Curtis method may be adopted. Specifically, let
\[ x_j = \cos(j\pi/n), \quad j = 0, 1, \ldots, n, \quad (2.3.7) \]
and
\[ p_k(x) = T_k(x), \quad k = 0, 1, \ldots, n, \quad (2.3.8) \]
where $T_k(x)$ denotes the Chebyshev polynomial of the first kind.

In practice there are good reasons to prefer the use of cosine-distributed points over the equal spaced points used by Levin. To see why this is the case, we first demonstrate that if the integration rule (2.3.1) is exact for the functions $f_k(x)$ with either choice of $p_k(x)$, then it is exact for any polynomial of degree $\leq n$. This establishes that the formula is a product integration rule of the interpolatory type. A number of well known theorems on the properties of interpolatory integration rules can then be used to show why the points (2.3.7) should be preferred to the equal spaced alternative.

**Lemma 2.1** If the integration rule (2.3.1) is exact for the functions (2.3.2) with $p_k(x) = x^k$ or $p_k(x) = T_k(x)$, then it is exact for any polynomial of degree $\leq n$.

**Proof.** If an integration rule of the form (2.3.1) is exact for a set of functions $f_k(x)$, then it is also exact for any linear combination of these functions. With $p_k(x) = x^k$ or $T_k(x)$ the functions $f_k(x) = i\tau p_k(x) + p_k(x)$, for $k = 0, 1, \ldots, n$, form a set of linearly independent polynomials of respective degree $k$, and so any polynomial of degree $\leq n$ is expressible as a linear combination of them. It follows that the integration rule is exact for any polynomial of degree $\leq n$. 
As the integration formula is interpolatory it is possible to give an explicit expression for the integration weights. Specifically,

\[ w_j = \int_{-1}^{1} \frac{\Pi(x)e^{ix\tau}}{\Pi(x_j)(x-x_j)} \, dx \]  

(2.3.9)

where

\[ \Pi(x) = (x-x_0) \cdots (x-x_n). \]  

(2.3.10)

In the particular case where the abscissae are spaced equally across the interval [-1,1], this simplifies to

\[ w_j = \frac{2e^{-i\tau}(-1)^{n-j}}{n!j!(n-j)!} \int_{0}^{1} \frac{x(x-1)(x-2) \cdots (x-n)e^{ix\tau/n}}{(x-j)} \, dx. \]  

(2.3.11)

For \( \tau = 0 \), which corresponds to the standard Newton-Cotes rules, Krylov [38] has given asymptotic representations of (2.3.11), which show that the integration weights become large and of mixed sign for increasing \( n \). It is not difficult to extend this analysis to give a similar result for the case of non-zero \( \tau \), with the implication that the integration rule (2.3.1) using equal spaced points is numerically unstable. For example, a small discrepancy in the values of \( f(x_j) \) can lead to a large error in the summation \( \sum w_j f(x_j) \). Integration weights that are large and of mixed sign also lead to loss of accuracy through subtractive cancellation, to an order equal to the magnitude of the largest weight. A derivation of the asymptotic expansions of the Newton Cotes integration weights for a weighted integral, which includes the case (2.3.11) for \( \tau \neq 0 \), is given by Kuz'min [54]. The asymptotic behaviour of Newton Cotes integration weights for weighted and non-weighted integrals is also considered by Davis and Rabinowitz [12, pp. 79-80] and Uspensky [80].

Krylov also gives a detailed discussion of the convergence of sequences of interpolatory rules and shows that it is the limiting distribution of the abscissae that determines the minimum region in which \( f(x) \) must be analytic for the process to converge. For equal spaced abscissae, convergence may only be guaranteed provided \( f(x) \) is analytic in a specific oval shaped region, the boundary of which is the level line of certain potential function. As a consequence, the process may fail to converge even if \( f(x) \) is analytic on the interval of integration.
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Clearly such a restriction, combined with the inherent numerical instability, means there is little or no benefit to be found in using the formula based on equal spaced points for large \( n \), and the alternative is to use the less efficient strategy of a low order rule combined with repeated subdivision.

In contrast, the cosine-distributed points are an optimal choice for use in interpolatory integration rules. Sloan and Smith [71] show that the integration rule (2.3.1), using the abscissae (2.3.7), will converge for any Riemann integrable function \( f(x) \). Furthermore the weights, whilst not necessarily all positive, exhibit some useful properties. In particular, the sum of their absolute values, \( \sum |w_j| \), is bounded and tends to the limit \( f_{-1}^1 |e^{irx}| \, dx \), which is the best possible in that any smaller limit would be inconsistent with the property of convergence for all continuous functions. The practical importance of this result lies in the guarantee of numerical stability as \( n \) increases. If each \( f(x_j) \) is in error by \( \epsilon \), then the maximum possible error in the integration sum is \( \epsilon \sum |w_j| \), which is always less than \( \epsilon f_{-1}^1 |e^{irx}| \, dx \). This is a significant improvement over the formula using equal spaced points, for which this sum grows without bound 1.

Although the above comments are only valid for \( q(x) = x \), they may be used as motivation when considering more general functions. Certainly the choice of equal spaced points, as made by Levin, has little to recommend it. On the other hand, the cosine-distributed abscissae would seem a natural choice, and in practice they prove remarkably more effective.

Hence, the recommended implementation is to make the integration rule

\[
\int_{-1}^{1} e^{irq(x)} f(x) \, dx \approx \sum_{j=0}^{n} w_j f(x_j)
\]

To prove this it is sufficient to note that for an interpolatory quadrature process to converge for any continuous function it is necessary and sufficient that \( \sum_{j=0}^{n} |w_j| \leq K < \infty \) for some number \( K \) with \( n = 0, 1, 2, \ldots \). However, as the equal spaced integration rule may fail to converge even for functions that are analytic on the interval, it follows that the sum \( \sum |w_j| \) is unbounded.
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exact for the functions

\[ f_k(x) = i \pi q'(x) p_k(x) + p_k'(x), \quad k = 0, 1, \ldots, n, \]  

(2.3.13)

with the abscissae \( x_j \) given by (2.3.7) and the functions \( p_k(x) \) by (2.3.8).

Before moving on to consider the practical use of the integration formula, it is worthwhile to point out that Sloan and Smith [75] have extended their results on convergence and numerical stability, to include the case where the abscissae are given by the roots of the Jacobi polynomial \( P_n^{(\alpha, \beta)}(x), (\alpha, \beta > -1) \). In principle therefore, the above comments for \( q(x) = x \) are valid for other sets of points, say the zeros of the Legendre polynomials. However, in practice the cosine-distributed points (2.3.7) have the advantage of being progressive when the order of the formula is doubled, allowing function evaluations to be re-used. They are also straightforward to compute for any value of \( n \), a property which isn't true for the zeros of the Jacobi polynomials.

2.4 Practical use of the rule

In order to illustrate the above points, the integration rule (2.3.12) using cosine-distributed abscissae and the Chebyshev polynomials \( T_k(x) \), has been applied to a typical problem from the test set of Section 2.5, and its effectiveness for increasing point number \( n \) has been compared to the same formula using equal spaced points and powers of \( x \).

Both variations have been applied to the evaluation of

\[ C(40, 0) = \frac{1}{\beta} \int_{0}^{\beta} \cos(40 \cos \theta) \cos \theta \, d\theta, \quad \beta = 0.72, \]  

(2.4.1)

which is a specific example of the general diffraction integral

\[ C(x, y, \beta) = \frac{1}{2\beta} \int_{-\beta}^{\beta} \cos(x \cos \theta - y \sin \theta) \cos \theta \, d\theta \]  

(2.4.2)

introduced in Chapter 1. These integrals are cited by Davis and Rabinowitz [12] as requiring special study and treatment, particularly for large \( x \) and \( y \).
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Table 2.1: The number of correct figures achieved in the evaluation of \( C(x, y, \beta) \) using the combination of (2.3.5) and (2.3.6) for the equal spaced formula, and equations (2.3.7) and (2.3.8) for the cosine based formula, as the point number \( n \) is increased.

\[
\begin{array}{ccc}
 n & \text{Equal} & \text{Cosine} \\
2 & 0 & 0 \\
4 & 1 & 0 \\
8 & 2 & 2 \\
16 & 7 & 10 \\
32 & 9 & 15 \\
64 & 7 & 15 \\
\end{array}
\]

Table 2.1 gives the number of correct figures achieved using the combination of (2.3.5) and (2.3.6) for the equal spaced formula, and equations (2.3.7) and (2.3.8) for the cosine based formula, as the point number \( n \) is increased. The values of \( n \) were chosen so that both formulas were progressive, allowing previously computed values of \( f(x) \) and \( q'(x) \) to be re-used at each stage. In each case, the integration weights were computed to machine accuracy, approximately 15 significant figures. Table 2.2 gives the absolute value of the maximum integration weight in the computed formulas, where the figure in brackets represents the exponent, for example 4.728(-1) represents \( 4.728 \times 10^{-1} \) or equivalently 0.4728. This convention is used in subsequent tables.

Despite the fact that the integration rule is no longer interpolatory, the difficulties associated with using equal spaced abscissae are still evident. The integration weights grow rapidly as the order \( n \) is increased and this accounts, in part, for the poor performance of the 32 point and 64 point formulas. As discussed in Section 2.3, integration weights that are large and of mixed sign are a recipe for numerical disaster, causing loss of accuracy through subtractive cancellation and by amplifying initial errors in the function values \( f(x_j) \). Numerical experience
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Table 2.2: The absolute value of the maximum integration weight in the computed formulas for the integral $C(x, y, \beta)$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>Equal</th>
<th>Cosine</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>4.728(-1)</td>
<td>4.728(-1)</td>
</tr>
<tr>
<td>4</td>
<td>7.090(-1)</td>
<td>7.363(-1)</td>
</tr>
<tr>
<td>8</td>
<td>5.025(-1)</td>
<td>3.982(-1)</td>
</tr>
<tr>
<td>16</td>
<td>7.409(+0)</td>
<td>1.896(-1)</td>
</tr>
<tr>
<td>32</td>
<td>2.734(+5)</td>
<td>9.562(-2)</td>
</tr>
<tr>
<td>64</td>
<td>4.984(+7)</td>
<td>1.118(-1)</td>
</tr>
</tbody>
</table>

suggests that this situation is typical, and that at $n = 32$ the maximum integration weight is of the order $10^5$. For $n = 64$ this value increases to $10^8$. On a machine employing 15 figure arithmetic this effect limits the obtainable accuracy to 10 and 7 figures respectively.

In contrast, the formula based on cosine-distributed abscissae performs significantly better, delivering 3 figures more accuracy than the equal spaced formula at $n = 16$ and five extra figures at $n = 32$, by which point the results are accurate to machine precision. Furthermore, the integration weights remain small in magnitude as $n$ increases and this helps to maintain the numerical stability of the formula, as illustrated by the result for $n = 64$.

As a final practical point it is important to discuss the computation of the integration weights, which are determined from a system of linear equations. As with many systems that arise in applications, the linear equations become ill-conditioned as $n$ increases, a fact that may be confirmed by computing the traditional condition number of the system. Some representative figures, from the current example, are presented in Table 2.3. As a consequence, determining the integration weights with any accuracy becomes extremely difficult for large values of $n$. For example, with point numbers above $n = 32$, LU decomposition
working to machine precision typically returns no correct figures. To overcome this problem there are a number of options available, for example the use of extended precision arithmetic, but these invariably require more computation than standard LU decomposition. Fortunately, by making use of a property of the LU algorithm, it is possible to avoid these more expensive alternatives. The principle relies on the following, almost obvious, lemma.

**Lemma 2.2** Denote the defining system of linear equations by

\[ Aw = b, \quad (2.4.3) \]

where

\[ b_k = \left[ e^{i\tau q(x)}p_k(x) \right]_{-1}^1, \quad k = 0, 1, \ldots, n, \]

\[ a_{k,j} = i\tau q'(x_j)p_k(x_j) + p_k'(x_j), \quad k, j = 0, 1, \ldots, n, \quad (2.4.4) \]

and \( w = (w_0, w_1, \ldots, w_n)^T \) is the vector of integration weights. Let \( w^* \) denote a computed solution of the system, obtained by whatever method, and define the residual vector as

\[ r = Aw^* - b. \quad (2.4.5) \]

Furthermore, let \( I_n \) represent the formula (2.3.12) using the integration weights \( w_j \) and \( J_n \) represent the same formula using the computed integration weights \( w_j^* \). Then \( |I_n - J_n| = |r_k| \) for the functions \( f_k(x) \) given by (2.3.2).

**Proof.** For the functions \( f_k(x) \) the quantities \( I_n \) and \( J_n \) are given by

\[ \sum_{j=0}^{n} w_j [i\tau q'(x_j)p_k(x_j) + p_k'(x_j)] \quad (2.4.6) \]

and

\[ \sum_{j=0}^{n} w_j^* [i\tau q'(x_j)p_k(x_j) + p_k'(x_j)] \quad (2.4.7) \]

respectively. It is clear that \( I_n \) is simply the \( k^{th} \) component of the product \( Aw \) and so, by construction, is equal to \( b_k \). In a similar manner \( J_n \) is the \( k^{th} \) component of \( Aw^* \) and is therefore equal to \( b_k + r_k \). Hence

\[ |I_n - J_n| = |b_k - (b_k + r_k)| = |r_k| \quad (2.4.8) \]
as required.

Now consider the quantity $|I_n - J_n|/|I_n|$. This is just the relative error incurred when $I_n$ is approximated by $J_n$, or alternatively the error incurred when the computed integration weights are used in place of the true integration weights. By the above lemma, for the functions $f_k(x)$, this ratio is equal to $|r_k|/|b_k|$. If this ratio can be made small, the computed solution will yield an integration formula which performs almost as well for the basis functions as the accurate solution. More precisely, if $|r_k|/|b_k| \leq \epsilon$, $k = 0, 1, \ldots, n$, where $\epsilon$ is $O(10^{-b})$, then for the functions $f_k(x)$, $I_n$ and $J_n$ will agree to $b$ decimal places. If $\epsilon$ can be reduced to the order of machine precision, then $I_n$ and $J_n$ will be exact for the same functions, at least to machine accuracy, and will produce almost indistinguishable results. It is well known, see Golub and Van Loan \cite{32} for instance, that standard LU decomposition with partial pivoting is a residual minimizing algorithm and is therefore an effective way to generate the integration weights. In practice, if $c$ is the vector with components $c_k = |r_k|/|b_k|$, then $\|c\|_{\infty}$ will be of the order of machine precision, and there will be no noticeable reduction in performance when weights computed in this manner are used in the integration formula.

To illustrate this argument, Table 2.3 gives the number of correct figures achieved when the integration rule employing the computed weights is applied to the current example. Also given is $\|c\|_{\infty}$, together with the condition number of the linear system, defined by $\kappa(A) = \|A\|_2 \|A^{-1}\|_2$. Only the results corresponding to the cosine-based formula are presented.

There are a number of points to note. For $n \leq 16$, LU decomposition returns accurate solutions so no differences between the above results and those in Table 2.1 should be expected. However, for $n = 32$ and $n = 64$, the condition numbers suggest severe ill-conditioning, and in both cases the computed solution contains no correct figures. Despite this, there is little or no reduction in performance noted by using the computed integration weights in place of the accurate weights, and this is due entirely to the small residuals, which as predicted are consistently
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<table>
<thead>
<tr>
<th>$N$</th>
<th>No. of figures</th>
<th>$|c|_\infty$</th>
<th>$\kappa(A)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0</td>
<td>3.390(-15)</td>
<td>9.495(00)</td>
</tr>
<tr>
<td>4</td>
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<td>3.271(00)</td>
</tr>
<tr>
<td>8</td>
<td>2</td>
<td>1.017(-15)</td>
<td>1.014(01)</td>
</tr>
<tr>
<td>16</td>
<td>10</td>
<td>2.664(-14)</td>
<td>3.904(03)</td>
</tr>
<tr>
<td>32</td>
<td>15</td>
<td>4.964(-14)</td>
<td>4.115(12)</td>
</tr>
<tr>
<td>64</td>
<td>15</td>
<td>8.398(-14)</td>
<td>3.275(14)</td>
</tr>
</tbody>
</table>

Table 2.3: The application of computed integration weights of the order of machine precision.

2.5 Examples and comparisons

The proposed method has been applied to a number of examples compiled from the work of Ehrenmark [16], Levin [41], Hartree [36] and Bakhvalov and Vasil'eva [7], together with some further integrals that exhibit particular difficulties. These are presented in Table 2.4.

Table 2.5 gives the number of function evaluations required to produce 15 figure accuracy for each integral. The triple $(n, 2, n)$ relating to $(f, q, q')$ means that the formula of order $n$ was required, which uses $n + 1$ evaluations of $f$ and $q'$, and two evaluations of $q$. For these examples, the order of the formula has been purposely limited to $n \leq 128$, as above this level the computation of the integration weights becomes a significant part of the overall computing time, rendering the usual measure of function counts less important. In practice, there is a need to balance the maximum order used against the time required to compute the integration weights, and much of this will depend on how computationally expensive the functions $f$, $q$ and $q'$ are to evaluate. For example, if these functions are straightforward to compute, it may be better to use a maximum order of $n = 48$ or $n = 64$, combined with some suitable subdivision strategy.
CHAPTER 2. IRREGULAR TRIGONOMETRIC INTEGRALS

<table>
<thead>
<tr>
<th>I</th>
<th>Integral</th>
<th>Value</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>I₁</td>
<td>( \int_{100}^{200}(1 + \ln x) \cos(x \ln x) , dx )</td>
<td>-1.77429897490598(-0)</td>
<td>Ehrenmark</td>
</tr>
<tr>
<td>I₂</td>
<td>( \int_{0}^{\beta} \cos x \cos(40 \cos x) / \beta , dx )</td>
<td>5.01944561062042(-2)</td>
<td>Hartree</td>
</tr>
<tr>
<td>I₃</td>
<td>( \int_{0}^{1} \sin x \cos(500(x^2 + x)) , dx )</td>
<td>4.5985939784012(-4)</td>
<td>Levin</td>
</tr>
<tr>
<td>I₄</td>
<td>( \int_{0}^{2\pi} \ln x \sin 30x , dx )</td>
<td>-1.93877275099872(-1)</td>
<td>Levin</td>
</tr>
<tr>
<td>I₅</td>
<td>( \int_{0}^{1} \cos x \cos(100\sqrt{1 - x^2}) , dx )</td>
<td>3.25497765499960(-2)</td>
<td>Present</td>
</tr>
<tr>
<td>I₆</td>
<td>( \int_{0}^{1} \sin(\frac{x}{1-x}) , dx )</td>
<td>3.43377961556427(-1)</td>
<td>Levin</td>
</tr>
<tr>
<td>I₇</td>
<td>( \int_{0}^{2} e^x \sin(50 \cosh x) , dx )</td>
<td>7.0765298761836(-2)</td>
<td>Present</td>
</tr>
<tr>
<td>I₈</td>
<td>( \int_{-1}^{1} \cos(\frac{47\pi x^2}{4}) \cos(\frac{45\pi x}{4}) , dx )</td>
<td>2.33286903629123(-3)</td>
<td>Bakhvalov</td>
</tr>
<tr>
<td>I₉</td>
<td>( \int_{0}^{1} e^{-\tan x \sec^2 x \cos(100 \tan x)} , dx )</td>
<td>9.99900000999900(-4)</td>
<td>Present</td>
</tr>
</tbody>
</table>

Table 2.4: Example integrals

The "Type" column indicates whether an open or closed formula was used to evaluate the integrals. For problems involving end-point singularities, the abscissae

\[ x_j = \cos \left( \frac{\pi (2j + 1)}{2(n + 1)} \right), \quad j = 0, 1, \ldots, n \]

(2.5.1)

were used in place of the points (2.3.7). In this case the results of Sloan and Smith [71] are still valid, but the abscissae have the advantage that they do not include the end-points -1 and 1. A further sets of points that may prove useful are the semi-open abscissae

\[ x_j = \cos \left( \frac{2j\pi}{2n + 1} \right), \quad j = 0, 1, \ldots, n \]

(2.5.2)

which exclude the end-point \( x = -1 \). These points are also covered by the results of Sloan and Smith.

In each of the examples presented here the integration weights were computed using LU decomposition and typically, for point numbers above \( n = 32 \), were incorrect in every digit. This was done to illustrate the use of computed weights on a large set of integrals. Any results quoted below for the equal spaced formula
CHAPTER 2. IRREGULAR TRIGONOMETRIC INTEGRALS

<table>
<thead>
<tr>
<th>( I ) (( f, q, q' ))</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>( I_1 ) (2,2,2)</td>
<td>closed</td>
</tr>
<tr>
<td>( I_2 ) (24,2,24)</td>
<td>closed</td>
</tr>
<tr>
<td>( I_3 ) (24,2,24)</td>
<td>closed</td>
</tr>
<tr>
<td>( I_4 ) (62,2,62)</td>
<td>closed</td>
</tr>
<tr>
<td>( I_5 ) (48,2,48)</td>
<td>closed</td>
</tr>
<tr>
<td>( I_6 ) (44,2,44)</td>
<td>open</td>
</tr>
<tr>
<td>( I_7 ) (42,2,42)</td>
<td>closed</td>
</tr>
<tr>
<td>( I_8 ) (89,2,89)</td>
<td>closed</td>
</tr>
<tr>
<td>( I_9 ) (90,2,90)</td>
<td>open</td>
</tr>
</tbody>
</table>

Table 2.5: Number of function evaluations required to evaluate \( I_k \) to 15 significant figures

were obtained using integration weights computed accurately to 15 significant figures.

Example \( I_1 \) was chosen to have \( f(x) = q'(x) \) so that an analytic integral was available. As a consequence, the proposed method integrates this exactly using just the two point formula. The significant point to note is that full machine accuracy is maintained for all point numbers up to and including \( n = 128 \), demonstrating the numerical stability of the formula for increasing values of \( n \). Using the formula based on equal spaced abscissae, the accuracy drops to only seven significant figures at \( n = 48 \), by which point the maximum integration weight is of the order \( 10^7 \). The remarks of the previous section regarding loss of significance in the integration sum are clearly illustrated in this example.

Integrals \( I_2 \) and \( I_3 \) present no particular difficulties. Both are evaluated to the required accuracy using just the 24 point formula. Use of equal spaced abscissae for the same point number gives 10 figure accuracy in each case. Even at relatively low point numbers the cosine-based formula is noticeably more accurate. As the
CHAPTER 2. IRREGULAR TRIGONOMETRIC INTEGRALS

point number is increased, the integration weights in the equal spaced formula increase in magnitude and as a result the accuracy of the formula is reduced. In contrast, the proposed method maintains 15 figure accuracy for all orders up to \( n = 128 \).

Example \( I_8 \) is more difficult to evaluate because \( f(x) = \cos\left(\frac{45\pi x}{4}\right) \) is also rapidly oscillatory. In this case a relatively high order formula \( (n = 89) \) is needed to obtain the required 15 significant figures. The equal spaced formula, on the other hand, never achieves more than 3 significant figures. For integrals like this, where \( f(x) \) is badly behaved, it is often necessary to use high order approximations to obtain the desired accuracy. In such cases the present method is particularly effective, as it is the only formula that remains numerically stable and accurate as the order is increased.

Integrals \( I_6 \) and \( I_9 \) arise when infinite range oscillatory integrals are transformed onto a finite range. Specifically

\[
I_6 = \int_0^\infty \frac{\sin x}{(1+x)^2} \, dx, \quad x = \frac{u}{1-u}, \tag{2.5.3}
\]

and

\[
I_9 = \int_0^\infty e^{-x} \cos 100x \, dx, \quad x = \tan u. \tag{2.5.4}
\]

For \( I_6 \) the transformed integrand has \( q(x) = x/(1 - x) \), which is singular and has a singular derivative at \( x = 1 \). As a consequence the integrand oscillates faster and faster as \( x \to 1 \). Example \( I_6 \) contains a further difficulty in that both \( f(x) \) and \( q(x) \) are singular at the right-hand limit of integration. In each case, an open formula has been applied to evaluate the integrals, which avoids the need to evaluate the integrand at the singular end-points. By using this approach, the required accuracy is obtained for \( I_6 \) and \( I_9 \) with the 44 point and 90 point formulas respectively. It is interesting to note that the use of an open set of abscissae with such a high degree of success is in contrast to the comments of Levin, who suggests that the end points of the interval should always be used. Provided that the abscissae are selected appropriately it appears that this need
not be the case.

On first appearance it may seem unusual that integrals $I_6$ and $I_9$ in their original forms are more difficult to evaluate than the transformed integrals, which oscillate increasingly rapidly as $x$ closes in on the end-point of the interval. The explanation comes from examining the contribution to the integral in the vicinity of the singularity. For the infinite range integrals the contribution of $\int_\eta^\infty$ will be negligible for large enough $\eta$. The transformation maps the interval $[\eta, \infty)$ to a small interval whose end point is the singularity of the transformed integrand. By using an open formula this difficult region is effectively ignored without sacrificing accuracy.

The final integrals are $I_4$ and $I_5$, which are the most difficult examples of the set. In the first case the non-oscillatory term, $f(x) = \ln x$, possesses a logarithmic singularity at the lower limit of integration, while in the second case $q(x) = (1 - x^2)^\frac{1}{2}$ has singular derivatives at both limits of integration. A straightforward application of the current method, with $n = 128$, produces $I_4 = -1.93878198847438(-1)$ and $I_5 = 3.25531023041669(-2)$, which are correct to only 5 and 3 figures respectively. For comparison, Levin achieves the same accuracy for $I_4$ using just 70 function evaluations of $f(x)$ and $q'(x)$, and 8 evaluations of $q(x)$. However, it should be noted that Levin introduces specific basis functions for use around the singularity, based on analysis of his differential equation. This gives an overhead that is difficult to quantify and in this light the quoted figure is quite competitive. It would also be feasible to use specific basis functions in the present method, but this kind of approach is only useful for particular integrals and it is perhaps better to introduce a general strategy to deal with singularities. An obvious approach is to use a transformation to remove the singularity, at least in the function and its immediate derivatives. For $I_4$ use of the transformation $x = t^m$ as in Evans, Forbes and Hyslop [25] results in

$$I_4 = \int_0^{(2\pi)^\frac{1}{m}} mx^{m-1} \ln(x^m) \sin(30x^m) \, dx,$$

(2.5.5)
which even for low values of $m$ gives excellent results. For example, using $m = 7$, which is the quoted value, fifteen figure accuracy is achieved at only $n = 62$. When this result is compared with Levin, the benefits are obvious. Over twice the accuracy is obtained for fewer function evaluations, without the need to choose specific basis functions. For $I_5$ the obvious transformation is $x = \cos u$ which gives

$$I_5 = \int_0^{\frac{\pi}{2}} \sin x \cos(\cos x) \cos(100 \sin x) \, dx. \quad (2.5.6)$$

The integrand is then well-behaved and use of the 48 point formula gives full machine accuracy. Transformations of this type are useful for alleviating a wide range of singular behaviour, including $x^{-\alpha}(1 - x)^{-\beta}$, $x^{-\alpha}\ln x^\beta$, etc. and, when combined with the stability and accuracy of the current method, form an efficient method for evaluating singular oscillatory integrals.
Chapter 3
Integration rules for general oscillatory integrals

3.1 Introduction

It is increasingly common in modern applications to encounter oscillatory integrals of the form

$$\int_a^b w(x)f(x) \, dx, \quad -\infty < a < b < \infty,$$

(3.1.1)
in which the oscillatory kernel is something other than a simple trigonometric function or a single Bessel function of a linear argument. For such integrals, very few numerical integration methods have been developed. The reasons for this are quite straightforward to explain. Almost any attempt to approximate $f(x)$ in the usual form

$$f(x) \approx \sum_{k=0}^n a_k \phi_k(x),$$

(3.1.2)
for some suitable choice of functions $\phi_k(x)$, results in a series of integrals

$$M_k = \int_a^b w(x)\phi_k(x) \, dx, \quad k = 0, 1, \ldots, n,$$

(3.1.3)
which are as difficult to evaluate as the original integral. In certain instances, it may be possible to evaluate (3.1.3) efficiently, perhaps analytically or maybe by developing a bespoke numerical method to compute the integrals, but the details
invariably depend on the particular form of $w(x)$. Even minor modifications of
the oscillatory term typically leave the suggested methods unsuitable for the new
integrals. A case in point is the extended Clenshaw-Curtis method for the Fourier
integral
\[ \int_{-1}^{1} e^{ix} f(x) \, dx, \quad (3.1.4) \]
where the integrals equivalent to (3.1.3) are given by
\[ \int_{-1}^{1} e^{ix} T_k(x) \, dx, \quad k = 0, 1, \ldots, n. \quad (3.1.5) \]
In this instance, none of the methods outlined in Evans and Webster [28] are
applicable if the oscillatory term is changed to the irregular trigonometric form
discussed in the previous chapter. Alternative techniques, such as integration be­
tween the local maxima, present their own particular difficulties. For example, to
split the integral (3.1.1) into a series of non-oscillatory subintegrals, it is necessary
to determine the zeros of $w'(x)$. In most cases this cannot be done analytically and
the zeros have to be computed using a numerical method. For many oscillatory
functions, computing the turning points numerically offsets any benefits achieved
by converting the integral into a series of non-oscillatory integrals, particularly as
the frequency of the oscillations increases.

The purpose of this chapter is to introduce a new class of numerical integration
formula that may be used to evaluate integrals of the form (3.1.1). The idea is
an extension of the method developed for irregular trigonometric integrals, and
involves constructing a set of functions $f_0(x), \ldots, f_n(x)$, for which the integrals
\[ M_k = \int_{a}^{b} w(x) f_k(x) \, dx, \quad k = 0, 1, \ldots, n, \quad (3.1.6) \]
can be evaluated analytically using simple closed form expressions. The integral
(3.1.1) is then approximated using the formula
\[ \int_{a}^{b} w(x) f(x) \, dx = \sum_{j=0}^{n} w_j f(x_j) + E(f), \quad (3.1.7) \]
where the integration weights are selected so that the error $E(f)$ is zero for the
functions $f_0(x), \ldots, f_n(x)$. In this case the weights are determined by solving the
system of linear algebraic equations

\[ \sum_{j=0}^{n} w_j f_k(x_j) = M_k, \quad k = 0, 1, \ldots, n. \]  \hfill (3.1.8)

In the next section it is shown how the functions \( f_k(x) \) may be constructed for integrals involving a single Bessel function of a nonlinear argument. Section 3.3 extends the ideas developed here to oscillatory functions that satisfy a second order linear differential equation. Section 3.4 introduces a further extension appropriate for weight functions that satisfy an ordinary linear differential equation of order \( m \geq 1 \). Some examples of weight functions that are encompassed by this method are given in Section 3.5. In Section 3.6 comparisons are made with an alternative approach due to Levin. Finally, a number of examples which illustrate the practical application of the method are discussed in Section 3.7.

3.2 Bessel integrals

Integrals involving Bessel functions are, with the exception of Fourier transforms, the most common form of oscillatory integral that arise in physics and applied mathematics. The basic form of such integrals is

\[ \int_{a}^{b} J_\nu(\tau x) f(x) \, dx, \quad -\infty < a < b < \infty, \]  \hfill (3.2.1)

where \( J_\nu(x) \) is the Bessel function of the first kind of order \( \nu \), and \( \tau \) is a parameter that represents the frequency of the oscillations.

The evaluation of Bessel integrals is usually performed using an extended Clenshaw-Curtis formula. The first stage of this method is to convert the integral (3.2.1) into an equivalent integral over \([-1, 1]\). This is accomplished using the transformation

\[ x = \frac{1}{2}(b - a)t + \frac{1}{2}(b + a) = mt + c, \]  \hfill (3.2.2)

which gives

\[ \int_{a}^{b} J_\nu(\tau x) f(x) \, dx = m \int_{-1}^{1} J_\nu(\tau mt + \tau c) f(mt + c) \, dt. \]  \hfill (3.2.3)
The function \( f(mt + c) \equiv F(t) \) is then approximated using the finite Chebyshev expansion

\[
F(t) \approx \sum_{k=0}^{n} a_k T_k(t),
\]

with

\[
a_k = \frac{2}{n} \left[ \sum_{s=0}^{n} F \left( \cos \frac{\pi s}{n} \right) \cos \frac{\pi k s}{n} \right],
\]

where the notation \( \sum'' \) indicates that both the first and last terms of the summation are halved. The auxiliary integrals

\[
M_k = \int_{-1}^{1} J_{\nu}(\tau mt + \tau c) T_k(t) \, dt, \quad k = 0, 1, \ldots, n,
\]

are then evaluated using either an eight-term recurrence relation [61], or by expanding the Chebyshev polynomials as powers of \( x \) and using rapidly converging infinite series to compute the resulting integrals [20].

If the basic integral (3.2.1) is changed to

\[
\int_{a}^{b} J_{\nu}(\tau x) f(x) \, dx,
\]

then the evaluation is no longer straightforward. Approximations based on Chebyshev polynomials or powers of \( x \) are not feasible, as the integrals equivalent to (3.2.6) cannot usually be computed either analytically or numerically. The question then arises as to how integrals of this form may be evaluated efficiently. One idea is to extend some of the methods applicable to irregular trigonometric integrals to the current case. Evans [20], for example, has adopted this approach and used the transformation \( y = q(x) \) to convert the integral into the equivalent form

\[
\int_{q(a)}^{q(b)} J_{\nu}(\tau y) \frac{f(q^{-1}(y))}{q'(q^{-1}(y))} \, dy.
\]

This integral is of the form (3.2.1) and may be evaluated using the extended Clenshaw-Curtis method. An alternative that hasn’t been considered previously, but is certainly feasible, is to use the expansion of \( f(x) \) in the form

\[
f(x) \approx q'(x) \sum_{k=0}^{n} a_k g_k(q(x)).
\]
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Substitution of (3.2.9) into (3.2.7) gives

$$\int_a^b J_\nu(\tau q(x)) f(x) \, dx \approx \sum_{k=0}^n a_k \int_{q(a)}^{q(b)} J_\nu(\tau q) g_k(q) \, dq,$$

(3.2.10)

where the integrals on the r.h.s. may again be evaluated using the extended Clenshaw-Curtis method.

As both these techniques have generalisations to Bessel integrals, it seems appropriate to ask whether the integration scheme developed in Chapter 2 can also be extended to the current case. It turns out that the method does have an obvious extension and, furthermore, all the properties that make the formula so effective for trigonometric integrals are preserved for nonlinear Bessel integrals.

The idea behind the method is to find a form of $f(x)$ that allows the integral (3.2.7) to be evaluated analytically. To do this, consider the ordinary differential equation satisfied by $y = J_\nu(\tau x)$

$$y'' + \frac{1}{x} y' + \left(\tau^2 - \frac{\nu^2}{x^2}\right) y = 0.$$  

(3.2.11)

Applying the change of variables $x = q(t)$, it is straightforward to show that the function $y = J_\nu(\tau q(t))$ satisfies the differential equation

$$y'' + \left(\frac{q'(t)}{q(t)} - \frac{q''(t)}{q'(t)}\right) y' + [q'(t)]^2 \left(\tau^2 - \frac{\nu^2}{[q(t)]^2}\right) y = 0.$$  

(3.2.12)

Now consider the inhomogeneous equation

$$z'' + \left(\frac{q'(t)}{q(t)} - \frac{q''(t)}{q'(t)}\right) z' + [q'(t)]^2 \left(\tau^2 - \frac{\nu^2}{[q(t)]^2}\right) z = g(t),$$  

(3.2.13)

where the function $g(t)$ is unspecified for the moment. Multiplying (3.2.13) by $y$ and (3.2.12) by $z$ and subtracting gives

$$z'y - zy'' + \left(\frac{q'(t)}{q(t)} - \frac{q''(t)}{q'(t)}\right) (z'y - zy') = yg(t).$$  

(3.2.14)

Letting

$$u = z'y - zy'$$  

(3.2.15)

yields the equivalent differential equation

$$u' + \left(\frac{q'(t)}{q(t)} - \frac{q''(t)}{q'(t)}\right) u = yg(t).$$  

(3.2.16)
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As (3.2.16) is a first order linear differential equation it may be integrated exactly.

Multiplying both sides of this equation by the integrating factor

\[ p(t) = \exp \left[ \int \frac{q'(t)}{q(t)} - \frac{q''(t)}{q'(t)} \, dt \right] \]
\[ = \exp [\ln q(t) - \ln q'(t)] \]
\[ = \frac{q(t)}{q'(t)}, \quad (3.2.17) \]
gives

\[ \left[ \frac{q(t)}{q'(t)} \right]' = \frac{q(t)}{q'(t)} y g(t). \quad (3.2.18) \]

Setting

\[ g(t) = \frac{q'(t)}{q(t)} f(t), \quad (3.2.19) \]

and integrating (3.2.18) leads to the result

\[ \frac{q(t)}{q'(t)} u = \frac{q(t)}{q'(t)} (z'y - z'y') = \int y f(t) \, dt. \quad (3.2.20) \]

Hence, if \( z(t) \) is a particular solution of the differential equation

\[ z'' + \left( \frac{q'(t)}{q(t)} - \frac{q''(t)}{q'(t)} \right) z' + [q'(t)]^2 \left( \tau^2 - \frac{\nu^2}{[q(t)]^2} \right) z = \frac{q'(t)}{q(t)} f(t) \quad (3.2.21) \]
then

\[ \int_a^b J_\nu(\tau q(t)) f(t) \, dt = \left[ \frac{q(t)}{q'(t)} \left[ z'(t)J_\nu(\tau q(t)) - z(t)J'_\nu(\tau q(t)) \right] \right]_a^b. \quad (3.2.22) \]

Alternatively, if the functions \( f_k(t) \) are defined by

\[ f_k(t) = \frac{q(t)}{q'(t)} z''_k + \left( 1 - \frac{q''(t) q(t)}{[q'(t)]^2} \right) z'_k + q'(t) \left( \tau^2 q(t) - \frac{\nu^2}{q(t)} \right) z_k, \quad (3.2.23) \]
for some suitable choice of \( z_k(t) \), then the integrals

\[ M_k = \int_a^b J_\nu(\tau q(t)) f_k(t) \, dt, \quad k = 0, 1, \ldots, n, \quad (3.2.24) \]
may be evaluated using the closed form expression (3.2.22).
3.3 Second order differential equations

It is obvious that the method just described for Bessel function integrals may be extended to any oscillatory weight function, provided that it satisfies a second order linear differential equation. Let \( y = w(x) \) satisfy the differential equation

\[
y'' + a_1(x)y' + a_0(x)y = 0, \tag{3.3.1}
\]

and define the associated inhomogeneous equation

\[
z'' + a_1(x)z' + a_0(x)z = g(x). \tag{3.3.2}
\]

Proceeding as in the previous section yields the formula

\[
p(x)[z'(x)y(x) - z(x)y'(x)] = \int y(x)f(x) \, dx, \tag{3.3.3}
\]

where \( p(x) \) is the integrating factor

\[
p(x) = \exp \left[ \int a_1(x) \, dx \right], \tag{3.3.4}
\]

and

\[
f(x) = g(x)p(x). \tag{3.3.5}
\]

Hence, if the functions \( f_k(x) \) are defined by

\[
f_k(x) = p(x)[z''_k + a_1(x)z'_k + a_0(x)z_k], \tag{3.3.6}
\]

then the integral \( M_k \) may be evaluated using the analytic result

\[
M_k = \int_a^b w(x)f_k(x) \, dx = [p(x)z'_k(x)w(x) - p(x)z_k(x)w'(x)]_a^b. \tag{3.3.7}
\]

Probably the most important oscillatory kernels that fall into this class, besides the Bessel functions already discussed, are real trigonometric functions and the product of trigonometric and Bessel functions. In the first case, the oscillatory function is defined by

\[
w(x) = \cos q(x) \text{ or } \sin q(x), \tag{3.3.8}
\]
and $y = w(x)$ satisfies the differential equation (3.3.1) with

$$a_1(x) = \frac{q''(x)}{q'(x)}, \quad (3.3.9)$$

$$a_0(x) = [q'(x)]^2. \quad (3.3.10)$$

Hence, the integrating factor is given by

$$p(x) = \exp \left[ - \int \frac{q''(x)}{q'(x)} \, dx \right]$$

$$= \exp \left[ - \ln q'(x) \right]$$

$$= \frac{1}{q'(x)} \quad (3.3.11)$$

Of course, integrals involving trigonometric functions may be evaluated using the method developed in Chapter 2, and it might seem that the formulation presented here offers no new benefits. However, in practice, using the real form of the trigonometric functions in place of the complex expression significantly reduces the number of arithmetic operations required to compute the integration weights. In the complex case the integration weights are determined from a system of $n + 1$ complex linear equations, or equivalently a system of $2n + 2$ real linear equations. The real form of the trigonometric functions leads to a system of $n + 1$ real linear equations. As the solution of a system of $m$ linear equations requires approximately $\frac{1}{3} m^3$ multiplications and divisions, using the real trigonometric functions reduces the number of arithmetic operations involved by a factor of eight. The offsetting disadvantage is that it is necessary to evaluate both the first and second derivatives of $q(x)$, meaning that an additional $n + 1$ function evaluations are needed in this case.

For the product of trigonometric and Bessel functions, $w(x)$ is defined by

$$w(x) = e^{i\eta(x)} J_\nu(q_2(x)). \quad (3.3.12)$$

In this case, $y = w(x)$ satisfies the differential equation (3.3.1) with

$$a_1(x) = \frac{q'_2(x)}{q_2(x)} - \frac{q''_2(x)}{q_2(x)} - 2i\eta'_1(x), \quad (3.3.13)$$
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\[ a_0(x) = \left[ q_1'(x) \right]^2 \left( 1 - \frac{\nu^2}{[q_2(x)]^2} \right) \]
\[ - i q_1'(x) \left( \frac{q_2'(x)}{q_2(x)} - \frac{q_2''(x)}{q_2(x)} \right) - [q_1'(x)]^2 - i q_1''(x), \quad (3.3.14) \]

which leads to the integrating factor

\[ p(x) = \exp \left( \int \left( \frac{q_2'(x)}{q_2(x)} - \frac{q_2''(x)}{q_2(x)} - 2i q_1'(x) \right) \, dx \right) \]
\[ = \exp \left( \ln q_2(x) - \ln q_2'(x) - 2i q_1(x) \right) \]
\[ = \frac{q_2(x)}{q_2'(x)} e^{-2i q_1(x)}. \quad (3.3.15) \]

3.4 Use of Lagrange’s identity

To extend the above approach to other oscillatory weight functions, in particular Fresnel functions and products of Bessel functions, it is necessary to make use of some results from the theory of ordinary differential equations, see Coddington and Levinson [11] and Ince [37].

Let \( w(x) \) be an oscillatory kernel that satisfies the linear ordinary differential equation of order \( m \)

\[ \mathcal{L}w \equiv a_m(x)w^{(m)} + a_{m-1}(x)w^{(m-1)} + \cdots + a_1(x)w' + a_0(x)w = 0, \quad (3.4.1) \]

where the coefficients \( a_j(x) \) are prescribed in advance and the superscript \( (k) \) denotes \( k^{th} \) order differentiation with respect to \( x \). It is intended to generate an integration rule

\[ \int_a^b w(x)f(x) \, dx = \sum_{j=0}^n w_j f(x_j) + E(f), \quad (3.4.2) \]

in which the error \( E(f) \) is zero for a set of functions \( f_0(x), \ldots, f_n(x) \). The integration weights then follow from the system of linear algebraic equations

\[ \sum_{j=0}^n w_j f_k(x_j) = M_k, \quad k = 0, 1, \ldots, n, \quad (3.4.3) \]

where the constants \( M_k \) are defined by

\[ M_k = \int_a^b w(x)f_k(x) \, dx. \quad (3.4.4) \]
The challenge is to choose the functions $f_k(x)$ so that these integrals may be evaluated explicitly.

To do this, construct the adjoint operator $\mathcal{M}$ of $\mathcal{L}$ according to the formula

$$\mathcal{M}z \equiv (-1)^m(a_m z)^{(m)} + (-1)^{m-1}(a_{m-1} z)^{(m-1)} + \cdots + (a_1 z)' + a_0 z.$$  \hspace{1cm} (3.4.5)

The Lagrange identity in the theory of linear differential equations then states

$$z\mathcal{L}w - w\mathcal{M}z = [Z(w, z)]',$$  \hspace{1cm} (3.4.6)

where $Z(w, z)$ is the bilinear concomitant, and is equal to

$$Z(w, z) = \sum_{r=1}^{m} \sum_{j+k=r-1} (-1)^b(a_r z)^{(k)} w^{(j)}.$$  \hspace{1cm} (3.4.7)

Integrating the Lagrange identity the following Green's formula is obtained

$$\int_a^b z\mathcal{L}w \, dx - \int_a^b w\mathcal{M}z \, dx = [Z(w, z)]_a^b.$$  \hspace{1cm} (3.4.8)

Setting $z = z_k(x)$ and using the fact that $\mathcal{L}w = 0$ gives the following result

$$\int_a^b w(x)\mathcal{M}z_k(x) \, dx = -[Z(w, z_k)]_a^b.$$  \hspace{1cm} (3.4.9)

Hence, if the functions $f_k(x)$ are taken to be $\mathcal{M}z_k(x)$, for some suitably chosen functions $z_k(x)$, then the integrals

$$\int_a^b w(x)f_k(x) \, dx, \quad k = 0, 1, \ldots, n,$$  \hspace{1cm} (3.4.10)

may be evaluated analytically, provided that $w(x)$ and it's derivatives up to and including order $m-1$, can be evaluated at the end-points $a$ and $b$ of the interval of integration.

In some cases, it may turn out that although the weight function $w(x)$ satisfies a homogeneous linear differential equation, it also satisfies a simpler inhomogeneous linear differential equation of lower order. For this reason the above method is modified slightly to deal with weight functions that satisfy an inhomogeneous linear differential equation.
Assume that the oscillatory function $w(x)$ satisfies the inhomogeneous linear differential equation of order $m$

$$Lw \equiv a_m(x)w^{(m)} + a_{m-1}(x)w^{(m-1)} + \cdots + a_1(x)w' + a_0(x)w = h(x),$$  \hspace{1cm} (3.4.11)

where the functions $a_j(x)$ and $h(x)$ are prescribed in advance. Substituting $z = z_k(x)$ and $Lw = h(x)$ into equation (3.4.8) gives the corresponding Green's formula

$$\int_a^b w(x) Mz_k(x) \, dx = -[Z(w, z_k)]_a^b + \int_a^b z_k(x) h(x) \, dx.$$  \hspace{1cm} (3.4.12)

Since $h(x)$ and $z_k(x)$ are almost always elementary, the integral on the r.h.s of (3.4.12) can usually be integrated exactly. Thus, the inhomogeneous case is no more difficult than the homogeneous case.

It is interesting to point out how the above method differs from the technique described in the previous section. In the previous approach the functions $f_k(x)$ are taken to be $Lz_k(x)$, and most of the detail of the method involves finding an integrating factor to make the operator $L$ self-adjoint. For second order linear differential equations such an integrating factor can always be found. However, this approach fails when $L$ cannot actually be expressed in self-adjoint form, as is the case for many higher order differential operators. The present method instead sets $f_k = Mz_k(x)$ and thus avoids the need to find integrating factors.

### 3.5 Example weight functions

In this section some examples of $w(x)$ and the associated $Lw$, $Mz$ and $Z(w, z)$ are presented. Note, that $L$ is not uniquely determined by $w(x)$, and only the self-adjoint or the near self-adjoint form of $L$ is given. The freedom to choose alternative forms of $L$ allows the generation of a number of different integration formulas, a point which is illustrated in Section 3.7. Note also that where the function $q(x)$ is introduced it is assumed to be monotone on the interval $[a, b]$.

**Example 1(a)** Trigonometric function (complex form).
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\[ w(x) = e^{ix}. \]
\[ \mathcal{L}w = w' - iw = 0. \]
\[ \mathcal{M}z = -z' - iz. \]
\[ Z(w, z) = wz. \]

**Example 1(b) Trigonometric function of \( q(x) \) (complex form).**

\[ q = q(x). \]
\[ w(x) = e^{iq}. \]
\[ \mathcal{L}w = w' - iq'w = 0. \]
\[ \mathcal{M}z = -z' - iq'z. \]
\[ Z(w, z) = wz. \]

**Example 2(a) Trigonometric function (real form).**

\[ w(x) = \sin x \text{ or } \cos x. \]
\[ \mathcal{L}w = w'' + w = 0. \]
\[ \mathcal{M}z = \mathcal{L}(z). \]
\[ Z(w, z) = w'z - wz'. \]

**Example 2(b) Trigonometric function of \( q(x) \) (real form).**

\[ q = q(x). \]
\[ w(x) = \sin q \text{ or } \cos q. \]
\[ \mathcal{L}w = (w'/q')' + q'w = 0. \]
\[ \mathcal{M}z = \mathcal{L}(z). \]
\[ Z(w, z) = (w'z - wz')/q'. \]

**Example 3(a) Bessel function.**

\[ w(x) = C_\nu(x) \text{ where } C \text{ stands for } J, Y, H^{(1)} \text{ or } H^{(2)}. \]
\[ \mathcal{L}w = (xw')' + (x - \nu^2/x)w = 0. \]
\[ \mathcal{M}z = \mathcal{L}(z). \]
\[ Z(w, z) = x(w'z - wz'). \]
Example 3(b)  Bessel function of \( q(x) \).

\[ q = q(x). \]
\[ w(x) = C_v(q) \text{ where } C \text{ stands for } J, Y, H^{(1)} \text{ or } H^{(2)}. \]
\[ \mathcal{L}w = (qw'/q')' + q'(q - \nu^2/q)w = 0. \]
\[ \mathcal{M}z = \mathcal{L}(z). \]
\[ Z(w, z) = q(w'z - wz')/q'. \]

Example 4(a)  Fresnel integral.

\[ S(x) = \int_0^x \sin(\frac{x}{2}t^2) \, dt \text{ and } C(x) = \int_0^x \cos(\frac{x}{2}t^2) \, dt. \]
\[ w(x) = S(x) \text{ or } C(x). \]
\[ \mathcal{L}w = w'' - w'/x + \pi^2 x^2 w' = 0. \]
\[ \mathcal{M}z = -z'' - z'/x + (-\pi^2 x^2 + 2/x^3)z' - (2\pi^2 x + 2/x^3)z. \]
\[ Z(w, z) = w''z + wz'' - z'w' + (z'w - zw')/x + (\pi^2 x^2 - 1/x^2)zw. \]

Example 4(b)  Fresnel integral of \( q(x) \).

\[ q = q(x). \]
\[ S(q) = \int_0^q \sin(\frac{x}{2}t^2) \, dt \text{ and } C(q) = \int_0^q \cos(\frac{x}{2}t^2) \, dt. \]
\[ w(x) = S(q) \text{ or } C(q). \]
\[ p = 1/q'. \]
\[ \mathcal{L}w = (pw')'/q - (pw')'/q + \pi^2 q^2 w' = 0. \]
\[ \mathcal{M}z = -(p(z')'/q + (-\pi^2 q^2 + 2/q^2)z' - (2\pi^2 q^2 q + 2q'/q^3)z. \]
\[ Z(w, z) = p^2(z''w + w''z - w'z') + p(wz' - zw')/q \]
\[ + pp'(wz' + zw') + (\pi^2 q^2 - 1/q^2)zw. \]

It should be clear from these examples, that if the weight function \( w(x) \) satisfies a linear differential equation of order \( m \), then \( w(q(x)) \) also satisfies a linear differential equation of order \( m \). The particular differential equation satisfied by the transformed function may be obtained from the equation satisfied by the original function by applying the substitution \( x = q(t) \). From this it can be seen why it is necessary to assume that \( q(x) \) is monotone on \([a, b]\), because if this is
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not the case the transformation \( x = q(t) \) with

\[
\frac{d}{dx} = \frac{1}{q'(t)} \frac{d}{dt}
\]  

(3.5.1)

introduces a singularity at some point in \([a, b]\), by virtue of the fact the \( q'(t) \) must vanish somewhere in this interval.

Another useful point to note, is that if the functions \( w_1(x) \) and \( w_2(x) \) satisfy linear differential equations of order \( l \) and \( m \) respectively, then the product \( w(x) = w_1(x)w_2(x) \) satisfies a linear differential equation of order \( lm \). The operators \( \mathcal{L} \) and \( \mathcal{M} \), and the bilinear concomitant \( Z(w, z) \), relevant to some commonly occurring oscillatory products are presented below. The formulas appropriate for other products of oscillatory functions may be constructed from the formulas of the individual factors.

**Example 5(a)** Bessel \( J_\nu(x) \times \) Bessel \( Y_\nu(x) \).

\[
w(x) = u(x)v(x) \quad \text{where} \quad u \text{ and } v \text{ are } J_\nu \text{ or } Y_\nu.
\]

\[
\mathcal{L} w = x^2 w'' + 3xw'' + (1 - 4\nu^2 + 4x^2)w' + 4xw = 0.
\]

\[
\mathcal{M} z = -\mathcal{L}(z).
\]

\[
Z(w, z) = x^2(zw'' + z''w) + x(zw' + z'w) - x^2z'w' + 4(x^2 - \nu^2)zw.
\]

**Example 5(b)** Bessel \( J_\nu(q(x)) \times \) Bessel \( Y_\nu(q(x)) \).

\[
w(x) = u(q)v(q) \quad \text{where} \quad u \text{ and } v \text{ are } J_\nu \text{ or } Y_\nu \text{ and } q = q(x).
\]

\[
P = q/q' \quad \text{and} \quad R = P^2/2.
\]

\[
\mathcal{L} w = 2Rw'' + 3R'w'' + [R'' + 4(q^2 - \nu^2)]w' + 4qq'w = 0.
\]

\[
\mathcal{M} z = -\mathcal{L}(z).
\]

\[
Z(w, z) = 2Rzw'' + z''w) + R'(zw' + z'w) - 2Rz'w' + 4(q^2 - \nu^2)zw.
\]

**Example 6(a)** Bessel \( J_\mu(x) \times \) Bessel \( Y_\nu(x) \) with \( \mu \neq \nu \).

\[
w(x) = u(x)v(x) \quad \text{where} \quad u \text{ is } J_\mu \text{ or } Y_\mu, \text{ and } v \text{ is } J_\nu \text{ or } Y_\nu.
\]

\[
k = \mu^2 + \nu^2 \quad \text{and} \quad c = \mu^2 - \nu^2.
\]

\[
\mathcal{L} w = x^3w^{(4)} + 6x^2w'''' + (7x - 2kx + 4x^2)w'' + (1 - 2k + 16x^2)w' + (8x + c^2/x)w = 0.
\]
$Mz = x^3 z^{(4)} + 6x^2 z''' + (7x - 2kx + 4x^3) z'' + (1 - 2k + 8x^2) z' + (c^2/x) z.$

$Z(w, z) = x^3 (zw''' - z''w - z'w'' + z'''w') + 3x^2 (zw'' - z''w) + (x - 2kx + 4x^3)(zw' - z'w) + 4x^2 zw.$

**Example 6(b)** Bessel $J_\mu(q(x)) \times$ Bessel $Y_\nu(q(x))$ with $\mu \neq \nu$.

$w(x) = u(q) v(q)$ where $u$ is $J_\mu$ or $Y_\mu$, $v$ is $J_\nu$ or $Y_\nu$ and $q = q(x)$.

$k = \mu^2 + \nu^2$ and $c = \mu^2 - \nu^2$, $p = 1/q'$.

$L_w = \frac{q}{p} (p(pw')')' + 6q^2 (p(pw')')' + (7q - 2kq + 4q^3)(pw')'
+(1 - 2k + 16q^2) w' + (8q/p + c^2/qp) w = 0.$

$Mz = q^3 (p(pz')')' + 6q^2 (p(pz')')' + (7q - 2kq + 4q^3)(pz')'
+(1 - 2k + 8q^2) z' + (c^2/qp) z.$

$Z(w, z) = q^3 [zp(pw')' - p(pz')'w - p^2 z'(pw')' + p^2 (pz')'w']
+3q^2 [z(pw')' - (pz')'w]
+[q - 2kq + 4q^3] p(zw' - z'w) + 4q^2 zw.$

**Example 7(a)** Trigonometric $e^{isx} \times$ Bessel $J_\nu(q(x))$ or $Y_\nu(q(x))$.

$w(x) = e^{isx} J_\nu(q(x))$ or $e^{isx} Y_\nu(q(x)).$

$p = e^{-2isx}.$

$L_w = pxw'' + p(1 - 2isx) w' + p[(t^2 x - \nu^2/x) - is - xs^2] w = 0.$

$Mz = L(z).$

$Z(w, z) = px (w'z - wz').$

**Example 7(b)** Trigonometric $e^{iq(x)} \times$ Bessel $J_\nu(q_2(x))$ or $Y_\nu(q_2(x))$.

$q_1 = q_1(x)$ and $q_2 = q_2(x)$.

$w(x) = e^{iq_1} J_\nu(q_2)$ or $e^{iq_1} Y_\nu(q_2)$.

$p = e^{-2iq_1}$ and $r = q_2/q_1^2$.

$L_w = prw'' + (pr' + p'r) w' + p[q_2'(q_2 - \nu^2/q_2) - iq_1 r' - r(q_1^2) - ir q_1^2] w = 0.$

$Mz = L(z).$

$Z(w, z) = pr (w'z - wz').$
Finally, the example below is included to illustrate the use of an inhomogeneous equation. In certain instances, where the weight function satisfies a homogeneous differential equation and an inhomogeneous differential equation, it may be advantageous to use the inhomogeneous form.

Example 8  Trigonometric \times Trigonometric (real form).

\[ w(x) = u(q)v(q) \text{ where } u \text{ and } v \text{ are sin or cos and } q = q(x). \]
\[ w(x) = \sin^2 q \text{ or } \cos^2 q. \quad (u = v) \]
\[ Lw = (w'/q')' + 4q'w = 2q'. \]
\[ Mz = L(z). \]
\[ Z(w, z) = (zw' - z'w)/q'. \]

This approach may be beneficial, because only one integral has to be computed, compared to the alternative of splitting the integral into two:

\[ 2 \int_a^b f(x) \sin^2 q(x) \, dx = \int_a^b f(x) \, dx - \int_a^b f(x) \cos^2 q(x) \, dx. \]

The second case, where \( u \neq v \), reduces to Example 2(b).

3.6 An alternative approach

An alternative method for evaluating oscillatory integrals, developed independently of the above approach, has recently been proposed by Levin [42]. The technique is suitable for a general class of rapidly oscillatory integrals of the form

\[ \int_a^b f^T(x)w(x) \, dx \equiv \int_a^b \langle f, w \rangle(x) \, dx, \quad (3.6.1) \]

where \( f(x) = [f_1(x), \ldots, f_m(x)]^T \) is an \( m \)-vector of non-rapidly oscillatory functions and \( w(x) = [w_1(x), \ldots, w_m(x)]^T \) is an \( m \)-vector of linearly independent rapidly oscillatory functions. The principle is to assume that \( w_1(x), \ldots, w_m(x) \) satisfy a system of ordinary linear differential equations of the form

\[ \mathcal{L}\mathbf{w} \equiv \mathbf{w}' - A(x)\mathbf{w} = 0, \quad (3.6.2) \]
where $A(x)$ is an $m \times m$ matrix of non-rapidly oscillatory functions. Then, if an $m$-vector $p(x) = [p_1(x), \ldots, p_m(x)]^T$ can be found such that

$$\langle p, w \rangle' = \langle f, w \rangle,$$

(3.6.3)

the integral (3.6.1) may be evaluated using

$$\int_a^b (f, w)(x) \, dx = \int_a^b \langle p, w \rangle'(x) \, dx = p^T(b)w(b) - p^T(a)w(a).$$

(3.6.4)

Expanding (3.6.3), and using (3.6.2), it turns out that $p(x)$ should satisfy

$$\langle p, w \rangle' = \langle p', w \rangle + \langle p, w \rangle = \langle p', w \rangle + \langle p, A w \rangle = \langle p' + A^T p, w \rangle = \langle f, w \rangle,$$

(3.6.5)

or, equivalently, $p(x)$ should be a solution of the system of ordinary linear differential equations

$$M^* p = p' + A^T(x)p = f(x).$$

(3.6.6)

Now, as $f$ and $A$ are non-rapidly oscillatory, the system (3.6.6) has a particular solution that is also non-rapidly oscillatory, and the idea is to obtain an approximation to this particular solution using a collocation technique. Specifically an $n$-point approximation to the solution of (3.6.6) is defined as

$$p^n(x) = [p_1^{(n)}(x), \ldots, p_m^{(n)}(x)]^T,$$

(3.6.7)

with

$$p_j^{(n)}(x) = \sum_{k=1}^n c_k^{(j)} u_k^{(j)}(x), \quad j = 1, 2, \ldots, m,$$

(3.6.8)

where the functions $u_k^{(j)}(x)$ are chosen to be slowly oscillatory. The coefficients $c_k^{(j)}$ are then fixed using the collocation conditions

$$M^* p^n(x_l) = f(x_l), \quad l = 1, 2, \ldots, n,$$

(3.6.9)

where the points $x_1, \ldots, x_n$ are spaced equally across the interval $[a, b]$. This leads to a system of linear algebraic equations of order $mn$ that can be used to compute the coefficients. The corresponding $n$-point approximation to the integral (3.6.1) is given by

$$\int_a^b (f, w)(x) \, dx \approx [p^{(n)}(b)]^T w(b) - [p^{(n)}(a)]^T w(a).$$

(3.6.10)
To illustrate the application of this approach, consider the evaluation of the linear Bessel integral

$$\int_a^b J_\nu(\tau x)f(x) \, dx.$$  \hspace{1cm} (3.6.11)

In this case, the basis of the method are the two differential recurrence relations

$$J_{\nu-1}'(x) = \left(\frac{\nu - 1}{x}\right) J_{\nu-1}(x) - J_\nu(x),$$ \hspace{1cm} (3.6.12)

$$J_\nu'(x) = J_{\nu-1}(x) - \frac{\nu}{x} J_\nu(x).$$ \hspace{1cm} (3.6.13)

From these relations it follows that the 2-vector function

$$w(x) = [J_{\nu-1}(\tau x), J_\nu(\tau x)]^T$$ \hspace{1cm} (3.6.14)

satisfies the system (3.6.2) with

$$A(x) = \begin{pmatrix} \frac{\nu - 1}{x} & -\tau \\ \tau & -\nu/x \end{pmatrix}.$$ \hspace{1cm} (3.6.15)

Hence, the $n$-point approximation to (3.6.11) is given by

$$\int_a^b J_\nu(\tau x)f(x) \, dx \approx \left[ p_1^{(n)}(b) J_{\nu-1}(\tau b) + p_2^{(n)}(b) J_\nu(\tau b) \right]$$

$$- \left[ p_1^{(n)}(a) J_{\nu-1}(\tau a) + p_2^{(n)}(a) J_\nu(\tau a) \right],$$ \hspace{1cm} (3.6.16)

where $p^{(n)}(x) = [p_1^{(n)}(x), p_2^{(n)}(x)]^T$ is the $n$-point approximation to the solution of (3.6.6), with $A(x)$ given by (3.6.15) and $f(x) = [0, f(x)]^T$.

It should be clear that this approach and the method developed in Section 3.4 are based on similar principles, in the sense that both introduce specific differential operators which allow the oscillatory integral to be integrated exactly. However, the motivations behind each method are quite disparate, and when this is taken into account it is not surprising that two distinct methods have been proposed. In the above approach, the problem of evaluating the oscillatory integral is replaced by the problem of finding a non-rapidly oscillatory solution of a system of linear ordinary differential equations, and this latter problem is solved using a collocation technique. This idea is in keeping with Levin’s original philosophy.
for trigonometric integrals. In contrast, the technique presented in Section 3.4 is motivated by a desire to construct a standard numerical integration rule of the form

$$\int_a^b w(x)f(x)\,dx \approx \sum_{j=0}^n w_j f(x_j), \quad (3.6.17)$$

where the integration weights are fixed by making the formula exact for a set of \(n+1\) functions \(\{f_k(x)\}\). In this respect, the differential operators \(L\) and \(M\) are introduced for the sole purpose of allowing the integrals

$$\int_a^b w(x)f_k(x)\,dx, \quad k = 0, 1, \ldots, n, \quad (3.6.18)$$

to be evaluated explicitly. Again, the philosophy behind the trigonometric formula is carried through to the extended integration rule.

From a computational perspective, each method has its own strengths and weaknesses. Levin’s method has the advantage that it does not require the computation of the adjoint operator \(Mz\) or the bilinear concomitant \(Z(w, z)\), which can be very complicated in many instances\(^2\). On the other hand, the choice of \(w(x)\) and the associated matrix \(A(x)\) appears to be more ad hoc in his approach. For example, in the case considered above the approximation relies on the specific recurrence relations (3.6.12) and (3.6.13), and if the weight function is changed to a Fresnel integral say, it is not immediately obvious what form \(w(x)\) and \(A(x)\) should take. In contrast it is usually a simple matter to determine the differential operator \(L\) for most oscillatory kernels that arise in practice. This point is particularly relevant for weight functions of the form \(w(x) = w_1(x)w_2(x)\), because in such instances there is a straightforward procedure for determining the operator \(L\) from the respective operators of \(w_1(x)\) and \(w_2(x)\). For Levin’s method, there appears to be no equivalent way to obtain the vector \(w(x)\) and the associated matrix \(A(x)\).

A further practical point concerns the background computation involved in

\(^2\)With the increasing availability of computer algebra systems this aspect becomes less of an issue.
computing the $n$-point approximation for each formula. In Levin's method the $n$-point approximation leads to a system of linear algebraic equations of order $mn$ for the collocation coefficients. For the equivalent $n$-point formula of Section 3.4 the integration weights are determined from a system of linear equations of order $n$. As the solution of a system of linear equations of order $k$ requires approximately $\frac{1}{3}k^3$ multiplications and divisions, using the latter method reduces the number of arithmetic operations required by a factor of $m^3$. Such a reduction can result in a significant decrease in overall computing time, especially if $m$ is large. For example, for the product $\int_a^b f(x)g(x)\,dx$ the matrix $A(x)$ is $3 \times 3$, and so Levin's method requires 27 times as many arithmetic operations as the current approach.

Before moving on to consider the practical implementation of the proposed integration formula, it is interesting to investigate further the relationship with Levin's method outlined above. Hence, consider the identity

$$\int_a^b w(x)Mz(x)\,dx = -[Z(w, z)]_a^b, \tag{3.6.19}$$

where it is assumed $Lw = 0$. In Section 3.4 the idea was to let $f_k = Mz_k$ and then use (3.6.19) to evaluate the integrals $\int_a^b w(x)f_k(x)\,dx$. An alternative way to view this identity, is that if $z(x)$ is a particular solution of the differential equation

$$Mz(x) = f(x), \tag{3.6.20}$$

then

$$\int_a^b w(x)f(x)\,dx = -[Z(w, z)]_a^b. \tag{3.6.21}$$

Using this formulation it is possible to obtain a formula that bears some resemblance to Levin's approximation. Specifically, define the $n$-point approximation $z^{(n)}(x)$ to the particular solution $z(x)$ by

$$z^{(n)}(x) = \sum_{k=1}^n a_k u_k(x), \tag{3.6.22}$$

where the functions $u_k(x)$ are slowly oscillatory, and where the coefficients $a_k$ are fixed by the collocation conditions

$$Mz^{(n)}(x_j) = f(x_j), \quad j = 1, 2, \ldots, n. \tag{3.6.23}$$
Then the $n$-point approximation to the integral is given by

$$\int_a^b w(x)f(x) \, dx = - \left[ Z(w, z^{(n)}(x)) \right]_a^b.$$  \hspace{1cm} (3.6.24)

In principle, if $u_k(x) = z_k(x)$, then the approximation (3.6.24) is equivalent to the numerical integration rule of the previous section, however the alternative formulation presented here may offer some benefits in particular situations \(^3\).

It is also possible to use the operator $\mathcal{L}$ to construct the vector $\mathbf{w}$ and the matrix $A(x)$, by converting the differential equation $\mathcal{L}w = 0$ into a system of first order linear differential equations in the usual way. Hence, if $w(x)$ satisfies the second order equation

$$\mathcal{L}w \equiv a_2(x)w'' + a_1(x)w' + a_0(x)w = 0$$  \hspace{1cm} (3.6.25)

set $w_1 = w$ and $w_2 = w'_1 = w'$, then

$$w'_1 = w_2$$
$$w'_2 = -a_1(x)w_2/a_2(x) - a_0(x)w_1/a_2(x).$$  \hspace{1cm} (3.6.26)

Thus $\mathbf{w} = [w_1(x), w_2(x)]^T$ satisfies $\mathbf{w}' = A(x)\mathbf{w}$ with

$$A(x) = \begin{pmatrix} 1 & 0 \\ -a_1(x)/a_2(x) & -a_0(x)/a_2(x) \end{pmatrix}.$$  \hspace{1cm} (3.6.27)

In practice, decomposing the operator $\mathcal{L}$ into a form suitable for Levin's method is not likely to prove beneficial, for the reasons already discussed. However, what is interesting, is that the approximation obtained with this form of $\mathbf{w}$ and $A(x)$ is very similar to the approximation (3.6.24), in as much that both explicitly contain $w(x)$ and its first $m - 1$ derivatives.

### 3.7 Numerical results

In order to illustrate the effectiveness of the proposed integration formula, the method has been applied to a selection of oscillatory integrals. The oscillatory

\(^3\)So far we have not come across an example where this is actually the case.
CHAPTER 3. GENERAL OSCILLATORY INTEGRALS

Table 3.1: No. of significant figures achieved in the evaluation of \( \int_1^2 J_0(\tau x)e^x \, dx \) using cosine-distributed points

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \tau = 1 )</th>
<th>( \tau = 10 )</th>
<th>( \tau = 100 )</th>
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</table>

kernels studied below represent a typical cross-section of the types of integral that arise in applications.

The simplest test was to evaluate

\[
\int_1^2 J_0(\tau x)e^x \, dx,
\]

for \( \tau = 1, 10, 100, 1000 \). In this case, \( w(x) \) is of the form \( J_v(\tau x) \), and the associated \( \mathcal{L}, \mathcal{M} \) and \( Z(w, z) \) are given by Example 3(a) in Section 3.5. Two sets of results are presented. The first were generated using \( z_k(x) = T_k(x) \) and the cosine-distributed points \( x_j = \cos \pi j/n \). The second results were obtained using \( z_k(x) = x^k \) with the equal spaced points \( x_j = -1 + 2j/n \). The purpose of this was to illustrate that, as in the trigonometric case, the accuracy of the method is significantly reduced if the basis functions and abscissae are not chosen appropriately. The results of applying each formula, with point numbers from \( n = 4 \) to \( n = 64 \), are presented in Tables 3.1 and 3.2 respectively. Note, that in each case the integral was first converted to an equivalent integral over \([-1, 1]\), using the transformation (3.2.2).

As can be seen, the cosine-based method proves particularly effective, especially for the highly oscillatory cases \( \tau = 100, 1000 \), which are the most difficult to evaluate using standard numerical integration rules. Typically, a relative accuracy of \( 10^{-15} \) (roughly 14 significant figures) is achieved with just 16 evaluations of \( f(x) \). Furthermore, the integration rule exhibits numerical stability for increasing
values of \( n \), as illustrated by the results for \( n = 32 \) and \( n = 64 \). In contrast, the equal spaced formula remains stable only for low point numbers, and an analysis of the integration weights confirms that the weights become large and of alternating sign as \( n \) increases, which leads to numerical instability along the lines discussed previously. However, even with this restriction, the equal spaced formula is an effective tool, although the cosine-based formula is always to be preferred, unless there is good reason to suppose otherwise.

An additional benefit of the current method, is that the related integral

\[
\int_1^2 Y_0(\tau x)e^x \, dx, \tag{3.7.2}
\]

can be computed with very little extra effort. To see why this is the case, consider the system of linear equations that is used to generate the integration formula i.e.

\[
Aw = b, \tag{3.7.3}
\]

where

\[
a_{k,j} = Mz_k(x_j), \quad j, k = 0, 1, \ldots, n, \tag{3.7.4}
\]

\[
b_k = -[Z(w, z_k)]_a^b, \quad k = 0, 1, \ldots, n, \tag{3.7.5}
\]

and \( w = [w_0, \ldots, w_n]^T \) is the vector of integration weights. From these equations, it is clear that if the differential equation \( Lw = 0 \) has \( m \) solutions, then the

<table>
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<th>( n )</th>
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<th>( \tau = 10 )</th>
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Table 3.2: No. of significant figures achieved in the evaluation of \( \int_1^2 J_0(\tau x)e^x \, dx \) using equal spaced points
matrix \( A \) is the same for all \( m \) solutions. It is only the vector \( b \) that is dependent upon the particular solution under consideration. Hence, in the above example, the functions \( J_0(\tau x) \) and \( Y_0(\tau x) \) both lead to the same matrix \( A \). Now, if the linear equations are solved using LU decomposition, and the decomposition is stored, then the same system with a different r.h.s vector can be solved using just an additional \( n^2 \) operations. Hence, the integration weights for the \( Y_0(\tau x) \) formula can be determined using just the same number of operations. Since LU decomposition is an \( O(n^3) \) process, it is comparatively inexpensive to obtain the integration weights in this second case. Of course, this principle holds for all instances of the current method, and is not specific to the Bessel functions considered here.

From a computational perspective there are a few other points to note. First, the results given above were obtained using integration weights computed with LU decomposition, and usually for \( n \geq 32 \) the computed weights deviated completely from the accurate solution. Nevertheless, such integration weights may still be employed effectively, and the reason for this follows the same argument as in Section 2.4. Another aspect, which depends upon the form of \( w(x) \), is the computation of the terms of the matrix \( A \) and the vector \( b \). In the case of the matrix \( A \), it is necessary to evaluate the functions \( z_k(x) \) and their derivatives, up to and including order \( m \), at the points \( x_0, \ldots, x_n \). How this is done will depend upon the particular functions used, but if the recommended choice \( z_k(x) = T_k(x) \) is taken, then the values may be computed using the recurrence relations

\[
T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x),
\]

with

\[
T_0(x) = 1, \quad T_1(x) = x,
\]

and

\[
\frac{d^l}{dx^l} T_n(x) = 2^{l-1}(l-1)!nC_n^l(x), \quad l = 1, 2, \ldots, n,
\]

where \( C_n^l(x) \) is the Gegenbauer polynomial [17, Vol. 2, Chap. X]. This makes the
computation straightforward, as the Gegenbauer polynomials also satisfy a three
term recurrence relation

\[(n + 1)C_{n+1}^\lambda(x) = 2(n + \lambda)x C_n^\lambda(x) - (n + 2\lambda - 1)C_{n-1}^\lambda(x), \quad \lambda \neq 0, \quad (3.7.9)\]

with \(C_0^\lambda(x) = 1\) and \(C_1^\lambda(x) = 2\lambda x\). In practice, the use of these relations is made
under the assumption that the original integral over \([a, b]\) is first transformed to
an equivalent integral over \([-1, 1]\).

For the vector \(\mathbf{b}\), the individual components are given by the bilinear con­
comitants

\[Z(w, z_k) = \sum_{r=1}^{m} \sum_{j+l=r-1} (-1)^j (a_r z_k)^{(l)} w^{(j)}, \quad k = 0, 1, \ldots, n, \quad (3.7.10)\]

and an additional requirement is to evaluate the oscillatory weight function \(w(x)\),
and its derivatives up to and including order \(m - 1\), at the end-points of the
interval of integration. Again, how this is achieved very much depends upon the
precise form of \(w(x)\). In the context of a simple Bessel integral, for example, both
\(J_\nu(\tau x)\) and \(J'_\nu(\tau x)\) are needed. The first of these is straightforward to compute
using any number of published algorithms, one such being [14] for integer \(\nu\) or
[19, Chap. 6] for general real \(\nu\). The derivative can then be determined using the
expression

\[J'_\nu(\tau x) = -\tau J_{\nu+1}(\tau x) + \frac{\nu}{x} J_\nu(\tau x). \quad (3.7.11)\]

In fact, the algorithm presented in [19, Chap. 6] returns the values of \(J_\nu, J'_\nu, Y_\nu, Y'_\nu\)
simultaneously, which is particularly useful in the current context, as the integra­
tion weights for both formulas can be computed together using the approach
outlined above. For other weight functions, such as the Fresnel Sine integral

\[w(x) = \int_0^x \sin \left( \frac{\pi t^2}{2} \right) dt, \quad (3.7.12)\]
similar numerical techniques have to be used. Actually, in this case the derivatives
are straightforward to evaluate as they are just combinations of trigonometric
functions and powers of \(x\). On the other hand, the Fresnel integral itself is less
straightforward to compute, although it is not especially difficult in comparison to other special functions. An effective algorithm to evaluate Fresnel integrals, which uses a power series expansion for small values of $x$, and a continued fraction expansion for larger values, is presented in [19, Chap. 6]. The continued fraction expansion is again useful in the present context, as it returns the Fresnel Sine and Cosine integrals simultaneously, so that both sets of bilinear concomitants can be evaluated together.

The important point to remember, is that the application of the proposed method depends upon being able to evaluate the derivatives of the oscillatory kernel, and some thought must be given to how this can be achieved in a stable and efficient manner. In this respect, it is useful to keep in mind that for products of functions, the derivatives of the product can always be evaluated as products of the derivatives of the individual terms. Hence, products of trigonometric functions, Bessel functions and Fresnel integrals, can be handled using a combination of the algorithms referenced above, and this is sufficient to encompass many of the oscillatory integrals which arise in practical applications.

For the integral (3.7.1), there are, in fact, other effective numerical integration schemes which may be used in place of the current method, the extended Clenshaw-Curtis formula outlined in Section 3.2 a particular case in point. For this reason, a second integral is introduced

$$\int_{1}^{2} J_{0}(\tau(x^2 + \cos x))(1 + x^2)^{-1} \, dx, \quad (3.7.13)$$

for which such methods are not applicable. This integral is of the form of Example 3(b) in Section 3.5, and the results of applying the cosine-based formula for $\tau = 50, 500, 5000, 50000$ are presented in Table 3.3. For display purposes the results are truncated to 10 significant figures, although for $n \geq 16$ a relative accuracy of $10^{-15}$ was achieved in each case. Again, the accuracy and numerical stability of the formula are well illustrated, particularly for the extreme frequencies $\tau = 5000$ and $\tau = 50000$.

Notice, that in this example the $n$ point formula not only requires $n + 1$
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<table>
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<td>-2.167065014(-8)</td>
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</table>

Table 3.3: The evaluation of \( \int_a^b J_0(\tau(x^2 + \cos x))(1 + x^2)^{-1} \, dx \)

evaluations of \(f\), but also \(n + 1\) evaluations of \(q, q'\) and \(q''\), where \(q = x^2 + \cos x\), leading to a total function count of \(4n + 4\). However, it is important to realise that the usual measure of function evaluations as a degree of efficiency of the integration rule is less clear cut in the current case, because as \(n\) increases the solution of the linear equations may consume a large proportion of the overall computing time. Whether this is the case, or not, depends on how computationally expensive the functions \(f, q, q'\) and \(q''\) are to evaluate for a given argument. If the functions are relatively inexpensive to evaluate, then the time required to compute the integration weights will probably be the most significant part of the calculation. However, if they are expensive to evaluate, the computation of the integration weights is likely to be less of an issue. In practice, there is need to balance these two aspects in order to achieve the most efficient calculation and to minimise the total computing time. For most integrals, a sensible approach is to employ a progressive sequence of rules up to a maximum order of \(n = 48\) or \(n = 64\), and combine this sequence with a suitable subdivision strategy.

A further aspect to consider, is how to apply the current method to the integral

\[
\int_a^b J_\nu(\tau q(x)) f(x) \, dx, \tag{3.7.14}
\]

when \(q'(x)\) is zero at \(x = a\) or \(x = b\). In this case, the formula cannot be used
directly, as the bilinear concomitant

\[
Z(w, z) = \frac{q(x)}{q'(x)} [J'_0(\tau q(x))z(x) - z'(x)J_\nu(\tau q(x))],
\]

(3.7.15)
is singular at the vanishing end-point. For such integrals there are two possible ways to proceed. One approach is to factor out the singularity from the quotient \( q(x)/q'(x) \), which works provided \( q(x) \) and \( q'(x) \) have a zero in common. Particular examples include \( q(x) = (x - a)^k \) and \( (b - x)^k \). However, this method only works when \( q(x) \) has a multiple zero at the end-points, and when \( q(x) \) is simple enough to allow the factoring to be done. An alternative strategy, is to integrate the interval close to the zero using a standard numerical integration rule and complete the remainder of the integration with the current method. This technique works well, because in the neighbourhood of the zero, \( q(x) \) is almost constant and the integral is no longer oscillatory.

As a particular example of this technique, the integral

\[
\int_0^2 J_1(\tau(x^2 \cosh x)) \cos (\sin x) \, dx,
\]

(3.7.16)

was considered. In this case \( q'(x) \) is zero at \( x = 0 \). Hence, it is not possible to apply the integration formula directly, as each of the functions \( Z(w, z_k) \) is singular at the origin. To overcome this difficulty, the interval was split into \([0, \epsilon]\) and \([\epsilon, 2]\), and the former region was integrated using the Clenshaw-Curtis integration rule on the entire integrand. The current method was then used to evaluate the integral over the remaining interval. With \( \tau = 200 \) and \( \epsilon = 0.1 \) the Clenshaw-Curtis formula gave 14 figure accuracy at 16 points with the value \( 2.68595650450(-2) \), and the current method yielded the same accuracy at \( n = 80 \) with the value \( 6.7081914573(-3) \), giving a final value of \( 3.35677565023(-2) \). With \( \tau \) increased to 2000, the respective counts were 32 and 88, with a final value of \( 1.06808032704370(-2) \).

It is interesting to note, that the alternative ways of evaluating this type of integral described in Section 3.2, also encounter difficulties with zeros of \( q'(x) \).
For example, the transformation \( y = q(x) \) yields the equivalent integral

\[
\int_{q(a)}^{q(b)} J_\nu(\tau y) \frac{f(q^{-1}(y))}{q'(q^{-1}(y))} dy,
\]

which is singular when \( q'(x) \) vanishes. In this case, the device of integrating close to the zero with a standard integration formula must also be used. The modified Clenshaw-Curtis method can then be applied to complete the integration. As a competitor to the current method, this approach does have the advantage that \( q''(x) \) is not required, although in most examples the inverse function will have be computed numerically, leading to significantly higher function counts for \( q(x) \) and \( q'(x) \).

The singular nature of the bilinear concomitant at zeros of \( q'(x) \) is not confined to Bessel functions of a nonlinear argument, but is a general feature of weight functions of the form \( w(q(x)) \), as illustrated by the examples in Section 3.5. Furthermore, zeros of \( q'(x) \) on the interval \([a, b]\) introduce singularities into the functions \( M_{\nu k}(x) \), which may lead to singularities in the terms of the matrix \( A \), if one of the points \( x_0, \ldots, x_n \) coincides with the zero. Hence, it is best to avoid applying the method over an interval which contains a zero of \( q'(x) \). For integrals where this behaviour occurs the following procedure may be used: Locate the stationary values and subdivide the integral into a series of integrals between these points. Each integral is then of the form described above, and may be handled in a similar fashion. If the function \( q(x) \) is monotone on \([a, b]\), the method can be applied directly, without concern for singularities.

The final oscillatory kernel considered is the Bessel-trigonometric product

\[
w(x) = e^{iq(x)} C_\nu(q_2(x)),
\]

where \( C_\nu(x) \) is either \( J_\nu(x) \) or \( Y_\nu(x) \). Integrals containing two distinct oscillatory terms are especially difficult to evaluate using conventional numerical integration schemes, and even many oscillatory integration methods struggle with this type of integral, as most take into account only one of the oscillating components. For
example, to evaluate the integral

\[ \int_a^b e^{i\varphi(x)} C_\nu(q_2(x)) g(x) \, dx, \]  

(3.7.19)

it may be possible to use the trigonometric formula of Section 2.3, provided that 
\( f(x) = C_\nu(q_2(x)) g(x) \) is only slowly oscillatory, but this approach runs into difficulty when the Bessel function \( C_\nu(q_2(x)) \) is rapidly oscillatory, as is the case with most integrals of this type which arise in practice. The corresponding integration formula for Bessel integrals encounters similar problems when the trigonometric term is rapidly oscillatory.

The particular integral considered was

\[ \int_{1/2}^1 \cos(\tau_1 \cos x) J_0(\tau_2 x(1 + x)) e^x \, dx, \]  

(3.7.20)

which was evaluated for \( \tau_1 = 10, 100, 1000 \), with \( \tau_2 \) equal to double \( \tau_1 \). Two sets of results are presented. The first were obtained using \( \mathcal{L} \), \( \mathcal{M} \) and \( Z(w, z) \) given by Example 7 in Section 3.5. The second set were obtained with

\[ \mathcal{L} w \equiv w'' + a_1(x) w' + a_0(x) w = 0, \]  

(3.7.21)

where \( a_1(x) \) and \( a_0(x) \) are given by equations (3.3.14) and (3.3.14) respectively. In this case, the adjoint differential equation is given by

\[ \mathcal{M} z = z'' + b_1(x) z' + b_0(x) z, \]  

(3.7.22)

where

\[ b_1(x) = - \left( \frac{q_2'(x)}{q_2(x)} - \frac{q''_2(x)}{q'_2(x)} - 2i q'_1(x) \right) \]  

(3.7.23)

\[ b_0(x) = \frac{[q'_2(x)]^2}{[q_2(x)]^2} \left( 1 - \frac{\nu^2}{[q_2(x)]^2} \right) - i q'_1(x) \left( \frac{q_2'(x)}{q_2(x)} - \frac{q''_2(x)}{q'_2(x)} \right) \]  

\[ - [q'_1(x)]^2 + i q''_1(x) + \left( \frac{q_2'(x) q''_2(x) - [q'_2(x)]^2}{[q_2(x)]^2} \right) \]  

\[ \left( \frac{q_2(x) q''_2(x) - [q'_2(x)]^2}{[q_2(x)]^2} \right), \]  

(3.7.24)
Table 3.4: Evaluation of $\int_{1/2}^{1/2} \cos(\tau_1 \cos x) J_0(\tau_2 x(1 + x)) e^x dx$ using $\mathcal{L}$, $\mathcal{M}$ and $Z(w, z)$ from Example 7, Section 3.5

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Table 3.5: Evaluation of $\int_{1/2}^{1/2} \cos(\tau_1 \cos x) J_0(\tau_2 x(1 + x)) e^x dx$ using equations (3.7.21)-(3.7.25) and the bilinear concomitant is equal to

$$Z(w, z) = (w'z - wz') + a_1(x)wz.$$  \hspace{1cm} (3.7.25)

As previously mentioned, $\mathcal{L}$ is not uniquely determined by $w(x)$ and the purpose here was to examine the methods sensitivity to the choice of $\mathcal{L}$. The results are presented in Tables 3.4 and 3.5.

Again, both integration rules demonstrate accuracy and numerical stability, particularly for large $n$. The second version proves marginally more effective than the first in terms of the relative accuracy achieved for a given point number, although this comes at the expense of evaluating $q''_2(x)$. In general, our experience shows that there is little sensitivity to the choice of $\mathcal{L}$ and that, unless there is
good reason to do otherwise, the self-adjoint or near self-adjoint form of $L$ should be used. This is usually the easiest to implement.

It is useful to note, that the comments made previously regarding the benefits of using the real form of the trigonometric functions in place of the complex form, are also relevant to products of oscillatory functions where one of the terms is trigonometric. By working entirely with real functions, the linear equations can be reduced from a complex system of order $n + 1$ (or a real system of order $2n+2$), to a real system of order $n+1$, with an associated saving in computational effort. However, this saving must be offset against the additional complexity introduced into the differential equation satisfied by the product. For example, if the oscillatory kernel has the form

$$w(x) = e^{i\alpha q_1(x)}w_1(q_2(x)) \cdots w_p(q_{p+1}(x)), \quad q_i = q_i(x),$$

(3.7.26)

where each $w_i(q_{i+1})$ satisfies a differential equations of order $m_i$, then $w(x)$ satisfies a differential equation of order $m_1 \cdots m_p$. If, however, the real functions are used instead, then the order of the differential equation satisfied by the product is doubled, by virtue of the fact that $\cos(q)$ and $\sin(q)$ satisfy a differential equation of order 2. As a result, the expressions for $L$, $M$ and $Z(w, z)$ are usually more complicated and involve higher derivatives of $q_1, \ldots, q_{p+1}$. Whether this negates the benefit gained from reducing the order of the linear equations depends upon how computationally expensive the derivatives are to evaluate.

There is one further aspect of integrals involving products that is worth considering. In previous examples, where the oscillatory kernel consisted of a single function of the form $w(\tau q(x))$, it is was possible to use the transformation $y = q(x)$ to convert the integral

$$\int_a^b w(\tau q(x))f(x) \, dx,$$

(3.7.27)

into the equivalent form

$$\int_{q(a)}^{q(b)} w(\tau y)\frac{f(q^{-1}(y))}{q'(q^{-1}(y))} \, dy.$$

(3.7.28)
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Hence, if a numerical integration method is available for the integral

\[ \int_a^b w(\tau x) f(x) \, dx \]  \hspace{1cm} (3.7.29)

the original integral may be evaluated indirectly, by applying the integration formula to the transformed integral. However, in the case of the product (3.7.26), this technique is no longer applicable and so, even if an efficient numerical integration scheme can be developed for the integral

\[ \int_a^b e^{i\alpha} J_\nu(\tau_2 x) f(x) \, dx, \]  \hspace{1cm} (3.7.30)

it does not immediately lead to a way to evaluate the integral considered above.
Chapter 4
Evaluating a class of singular oscillatory integrals

4.1 Introduction

The numerical integration schemes developed in the previous chapters are effective for evaluating a wide class of oscillatory integrals. However, these methods should not disguise the fact that there are still a large number of oscillatory integrals which remain difficult to evaluate accurately and efficiently. The most important examples are integrals of the form

\[ \int_a^b w(x)f(x) \, dx, \]  

(4.1.1)

in which \( f(x) \) is singular at one or both end-points of the interval \([a, b]\), and where \( w(x) \) is the usual oscillatory weight function. In fact, integrals in which \( f(x) \) is continuous, but where the first or second derivatives are singular, also cause difficulties and fall into the category of difficult to evaluate.

For such integrals there are a number of possible avenues to pursue. The simple-minded approach is to ignore the singularity and apply an open integration formula, that is a method that doesn't employ the values of \( f(x) \) at \( x = a \) or \( x = b \).
CHAPTER 4. SINGULAR OSCILLATORY INTEGRALS

This was the first method used to evaluate the integral

\[ \int_0^{2\pi} \ln x \sin 30x \, dx, \quad (4.1.2) \]

in Section 2.5, and although a relative accuracy of $10^{-6}$ was obtained, this required the use of the 128 point formula. A better idea is to use a transformation to remove the singularity, at least in the function and its immediate derivatives. For example, for singularities of the form $x^\alpha$ or $x^\alpha \ln x$, with $\alpha > -1$, using the transformation $x(t) = t^n$ for large integer $n$, is usually sufficient to alleviate the effect of the singularity to a level which no longer causes difficulties. In the case of the above integral, using this transformation with $n = 7$ enabled 15 figure accuracy to be achieved using just the 62 point formula. A further approach is to integrate the region close to the singularity using a routine designed for singular integrals and then evaluate the remaining oscillatory integral using an oscillatory integration scheme. Hence, assuming that $f(x)$ is singular at $x = a$, the singular oscillatory integral is split into the equivalent form

\[ \int_a^b w(x)f(x) \, dx = \int_a^{a+\epsilon} w(x)f(x) \, dx + \int_{a+\epsilon}^b w(x)f(x) \, dx, \quad (4.1.3) \]

and the first integral on the r.h.s is evaluated using one of the methods described in Evans [21, Chap. 5] or Davis and Rabinowitz [12, pp. 172-190], and the second integral is computed using an appropriate oscillatory method, say the technique of Section 3.4.

In practice, each of these suggestions has its own strengths and weaknesses. The approach of ignoring the singularity is straightforward to apply provided that an open integration formula is available. One way to generate an open formula, is to use the method of the previous chapter in conjunction with the set of abscissae $x_j = \cos \pi(2j + 1)/(2(n + 1))$, $j = 0, 1, \ldots, n$, which are open on the transformed interval $[-1,1]$. However, ignoring the singularity is not a particularly effective method when the oscillatory term is absent, and it appears to be little more effective if the oscillatory term is present.
The use of a transformation to remove the singularity is a more efficient technique, as demonstrated by the example above, but there may be practical difficulties involved in implementing this approach for specific combinations of transformation and oscillatory kernel. To see why this is so, consider the integral

\[ \int_0^1 J_v(\tau x) f(x) \, dx. \quad (4.1.4) \]

In this case, the transformation \( x(t) = t^n \) leads to the equivalent integral

\[ \int_0^1 J_v(\tau t^n) n t^{n-1} f(t^n) \, dt, \quad (4.1.5) \]

and hence the method of the previous chapter cannot be applied directly to evaluate this, because the function \( q(t) = \tau t^n \) has a first derivative which is zero at \( x = 0 \), with the implication that the bilinear concomitant is singular at this point. However, in this instance \( q(x) \) is simple enough to allow the singularity to be cancelled from the quotient \( q(x)/q'(x) \) and the method can be applied in the usual manner. For more general transformations, though, this typically isn't the case. This is true for the transformation

\[ x(t) = cB_t(m, n), \quad c = 1/B(m, n), \quad (4.1.6) \]

where \( B_t(m, n) \) is the incomplete beta function defined by

\[ B_t(m, n) = \int_0^t t^{n-1}(1 - t)^{m-1} \, dt, \quad (4.1.7) \]

and \( B(m, n) \) is the standard beta function [19, Chap. 6]. This transformation is effective when \( f(x) \) is singular at both \( x = 0 \) and \( x = 1 \), because the derivative of the transformation, \( x'(t) = c t^{n-1}(1 - t)^{m-1} \), dampens the effect of the singularities at the end-points. Unfortunately, it is this property which prevents the oscillatory integration formula from being employed directly and, unlike the simple transformation \( x(t) = t^n \), it is not possible to factor out the singular points from the quotient \( q(x)/q'(x) \). The alternative is to apply the device suggested previously i.e. integrate close to the troublesome points using a standard numerical integration rule and complete the integration using the oscillatory integration formula.
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The final technique is similar in principle to the method just described. Hence, if the function \( f(x) \) is singular at \( x = a \), the interval is split into two intervals \( [a, a + \epsilon] \) and \( [a + \epsilon, b] \), and the integration over the former region is performed using an integration rule tailored to singular functions, and the integral over the latter region is evaluated using an oscillatory integration scheme. The basic idea is that if the integrand exhibits two distinct types of behaviour, then each should be handled using an appropriate type of formula. The main shortcoming of this technique, is that if \( \epsilon \) is too small the integrand remains close to singular on the range \( [a + \epsilon, b] \), resulting in an inefficient computation on the part of the oscillatory integration rule. Similarly, if \( \epsilon \) is too large, the integrand still exhibits rapidly oscillatory behaviour on the range \( [a, a + \epsilon] \), reducing the effectiveness of the singular integration routine.

In practice, the most efficient of the three techniques just described is the transformation approach, combined with the integration rule of Section 3.4. However, for specific types of singular behaviour, a more effective alternative is to factor out the singular term from the function \( f(x) \) and construct a numerical integration formula relevant to the particular combination of singular and oscillatory functions. Hence, if \( f(x) = h(x)g(x) \), where \( h(x) \) is the singular component and \( g(x) \) is assumed smooth, then a numerical integration formula is sought for the integral

\[
\int_a^b w(x)h(x)g(x) \, dx = \int_a^b k(x)g(x) \, dx, \quad k(x) = w(x)h(x).
\]  

(4.1.8)

An ideal way to do this, is to construct a product integration rule in the Clenshaw-Curtis style. However, as already noted in the previous chapters, almost any attempt to approximate \( g(x) \) by a series of Chebyshev polynomials results in a series of integrals which are as difficult to evaluate as the original integral. This is certainly the case when the singular term is absent, and the situation is not improved by the presence of the singular function. Nevertheless, for certain combinations of singular and oscillatory kernels, it is possible to evaluate the necessary integrals in a stable and efficient manner. In particular, for the singular...
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Fourier integral
\[ \int_a^b e^{irx} h(x)g(x) \, dx, \quad -\infty < a < b < \infty, \quad (4.1.9) \]

where \( h(x) \) has the form
\[ h(x) = \left[ \ln(b - x) \right]^r (b - x)^\alpha (x - a)^\beta \left[ \ln(x - a) \right]^s, \quad r, s = 0, 1, \quad (4.1.10) \]

with \( \alpha, \beta > -1 \), it is possible to generate an extended Clenshaw-Curtis formula by using a combination of Neumann series and asymptotic expansions to evaluate the required integrals.

In the next section the basic details of this method are discussed. Section 4.3 deals with the evaluation of singular Fourier integrals where only algebraic singularities are present. Extensions to the combination of algebraic and logarithmic singularities are considered in Section 4.4. Some numerical examples illustrating the application of the method are given in Section 4.5.

4.2 Singular Fourier integrals

The first stage of the method is to transform the singular Fourier integral (4.1.9) into an equivalent integral over \([-1,1]\). This may be accomplished using the transformation
\[ x = \frac{1}{2}(b - a)t + \frac{1}{2}(b + a) = mt + c, \quad (4.2.1) \]

which gives
\[
\int_a^b e^{irx} h(x)g(x) \, dx = \int_{-1}^1 e^{irmt+c} h(mt + c)g(mt + c) \, mdt
= K \int_{-1}^1 e^{im\Omega} H(t)G(t) \, dt, \quad (4.2.2)
\]

where \( \Omega = m\tau, G(t) = g(mt + c), H(t) = h(mt + c) \) and \( K = me^{irc} \). The function \( G(t) \) is then approximated using the finite Chebyshev expansion
\[
G(t) \approx \sum_{k=0}^n a_k T_k(t), \quad (4.2.3)
\]
where the coefficients \( a_k \) are given by
\[
a_k = \frac{2}{n} \left[ \sum_{\ell=0}^{n} G \left( \cos \frac{\pi s}{n} \cos \frac{\pi k s}{n} \right) \right], \quad k = 0, 1, \ldots, n. \tag{4.2.4}
\]

The resulting numerical integration formula can then be expressed as
\[
\int_{a}^{b} e^{irx} h(x) g(x) \, dx \approx \frac{2K}{n} \sum_{k=0}^{n} \left[ \sum_{s=0}^{n} G \left( \cos \frac{\pi s}{n} \cos \frac{\pi k s}{n} \right) \right] M_k(\Omega), \tag{4.2.5}
\]
where
\[
M_k(\Omega) = \int_{-1}^{1} e^{i\alpha x} H(x) T_k(x) \, dx, \quad k = 0, 1, \ldots, n. \tag{4.2.6}
\]
The main task is then to compute the integrals \( M_k(\Omega) \) in an accurate and efficient manner. By expanding the logarithms in the function \( H(x) \)
\[
H(x) = (\ln (m - mx))^{r}(m - mx)^{\alpha}(m + mx)^{\beta}(\ln (m + mx))^{s}
\]
\[
= (\ln m + \ln (1 - x))^{r} m^{\alpha+\beta}(1 - x)^{\alpha}(1 + x)^{\beta}(\ln m + \ln (1 + x))^{s},
\]
the integrals (4.2.6) can in turn be reduced to a sum of integrals of the form
\[
M_k(\alpha, \beta, r, s, \tau) = \int_{-1}^{1} e^{irx}[\ln(1 - x)]^{r}(1 - x)^{\alpha}(1 + x)^{\beta}[\ln(1 + x)]^{s}T_k(x) \, dx. \tag{4.2.7}
\]
It is the evaluation of this last set of integrals which is the concern of the next two sections.

### 4.3 Dealing with algebraic singularities

In this section it is shown how the integrals
\[
M_k(\alpha, \beta, \tau) = \int_{-1}^{1} e^{irx}(1 - x)^{\alpha}(1 + x)^{\beta}T_k(x) \, dx, \tag{4.3.1}
\]
can be evaluated accurately and efficiently by using a combination of Neumann series and asymptotic expansions.

The Neumann series approach is an extension of the method of Piessens and Poleunis [62] for the non-singular Fourier integral. The principle is to use the expansion
\[
e^{irx} = 2 \sum_{j=0}^{\infty} i^j J_j(\tau) T_j(x), \tag{4.3.2}
\]
which, upon substitution into (4.3.1), leads to the following Neumann series

\[ M_k(\alpha, \beta, \tau) = 2 \sum_{j=0}^{\infty} i^j J_j(\tau) R_{j,k}, \quad (4.3.3) \]

for the required integrals, where the notation \( \sum' \) indicates that the first term of
the summation is halved. The coefficients \( R_{j,k} \) are given by

\[ R_{j,k} = \int_{-1}^{1} (1 - x)^{\alpha}(1 + x)^{\beta} T_j(x)T_k(x) \, dx, \quad (4.3.4) \]

which, using the relation,

\[ T_j(x)T_k(x) = \frac{1}{2} [T_{j+k}(x) + T_{|j-k|}(x)], \quad (4.3.5) \]

may be expressed as

\[ R_{j,k} = \frac{1}{2} [N_{j+k} + N_{|j-k|}], \quad (4.3.6) \]

where

\[ N_n = \int_{-1}^{1} (1 - x)^{\alpha}(1 + x)^{\beta} T_n(x) \, dx. \quad (4.3.7) \]

For the original case considered by Piessens and Poleunis \((\alpha = \beta = 0)\), the
integrals \( N_n \) are easy to evaluate

\[ N_n = \begin{cases} 
0 & \text{n odd,} \\
-2/(n^2 - 1) & \text{n even,} 
\end{cases} \quad (4.3.8) \]

which gives

\[ R_{j,k} = \frac{1}{1 - (j + k)^2} + \frac{1}{1 - (j - k)^2}. \quad (4.3.9) \]

In the present case, the situation is slightly more complicated in that no simple
closed form is available. However, the integrals \( N_n \) can still be easily evaluated
by applying the results of the following lemma:

**Lemma 4.1** Let \( N_n \) be defined as in (4.3.7). Then the following recurrence relation holds for \( n \geq 1 \),

\[ (n/2+1+\alpha/2+\beta/2)N_{n+1} - (\beta - \alpha)N_n - (n/2-1-\alpha/2-\beta/2)N_{n-1} = 0, \quad (4.3.10) \]
where

\[ N_0 = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}, \quad (4.3.11) \]

\[ N_1 = \frac{2^{\alpha+\beta+1}(\beta-\alpha)\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+3)}. \quad (4.3.12) \]

**Proof.** Define \( h(x) \) as

\[ h(x) = (1-x)^\alpha(1+x)^\beta, \quad (4.3.13) \]

then

\[ (1-x^2)h'(x) = [(\beta-\alpha) - (\beta+\alpha)x]h(x). \quad (4.3.14) \]

It follows that

\[ \int_{-1}^{1} (1-x^2)h'(x)T_n(x) \, dx = \int_{-1}^{1} [(\beta-\alpha) - (\beta+\alpha)x]h(x)T_n(x) \, dx. \quad (4.3.15) \]

Denote the l.h.s integral by \( I_L \) and the r.h.s integral by \( I_R \). First consider \( I_R \),

\[ I_R = (\beta-\alpha) \int_{-1}^{1} h(x)T_n(x) \, dx - (\beta+\alpha) \int_{-1}^{1} h(x)xT_n(x) \, dx \quad (4.3.16) \]

\[ = (\beta-\alpha)N_n - (\beta+\alpha) \int_{-1}^{1} h(x)xT_n(x) \, dx. \quad (4.3.17) \]

If the three term recurrence relation satisfied by the Chebyshev polynomials is re­arranged to express \( xT_n(x) \) in terms of \( T_{n+1}(x) \) and \( T_{n-1}(x) \), the following formula is obtained

\[ xT_n(x) = \frac{1}{2}[T_{n+1}(x) + T_{n-1}(x)]. \quad (4.3.18) \]

Substituting this last expression into (4.3.17) produces the result

\[ I_R = (\beta-\alpha)N_n - \frac{1}{2}(\beta+\alpha)[N_{n+1} + N_{n-1}]. \quad (4.3.19) \]

Now consider the integral \( I_L \). Integration by parts gives

\[ I_L = \int_{-1}^{1} (1-x^2)T_n(x)h'(x) \, dx = [h(x)(1-x^2)T_n(x)]_{-1}^{1} - \int_{-1}^{1} h(x)((1-x^2)T_n'(x) - 2xT_n(x)) \, dx. \quad (4.3.20) \]

The bracketed term on the r.h.s vanishes at the limits of integration to leave only

\[ I_L = \int_{-1}^{1} h(x)[2xT_n(x) - (1-x^2)T_n(x)] \, dx. \quad (4.3.21) \]
Applying the relation

\[(1 - x^2)T'_n(x) = n[T_{n-1}(x) - xT_n(x)],\]

and rearranging the result, leads to the expression

\[I_L = \int_{-1}^{1} h(x)[(2 + n)xT_n(x) - nT_{n-1}(x)] \, dx.\]  

(4.3.23)

Using the formula for \(xT_n(x)\) in terms of \(T_{n+1}(x)\) and \(T_{n-1}(x)\) gives

\[I_L = \int_{-1}^{1} h(x) \left[ \left(1 + \frac{n}{2}\right)T_{n+1}(x) + \left(1 + \frac{n}{2}\right)T_{n-1}(x) - nT_{n-1}(x) \right] \, dx,\]  

(4.3.24)

which may be expressed as

\[h = \frac{(1 + \frac{n}{2})N_{n+1} + (1 + \frac{n}{2})N_{n-1} - nN_{n-1}}{(1 + n/2)N_{n+1} + (1 - n/2)N_{n-1}}.\]  

(4.3.25)

Combining the expressions for \(I_L\) and \(I_R\) gives

\[\left(1 + \frac{n}{2}\right)N_{n+1} + \left(1 - \frac{n}{2}\right)N_{n-1} = (\beta - \alpha)N_n - \frac{1}{2}(\beta + \alpha)[N_{n+1} + N_{n-1}],\]  

(4.3.26)

which can be rearranged into the form

\[(n/2 + 1 + \alpha/2 + \beta/2)N_{n+1} - (\beta - \alpha)N_n - (n/2 - 1 - \alpha/2 - \beta/2)N_{n-1} = 0,\]  

(4.3.27)

as required.

The expressions for \(N_0\) and \(N_1\) are straightforward to derive using the beta function. In the first case the original integral is given by

\[N_0 = \int_{-1}^{1} (1 - x)^\alpha(1 + x)^\beta T_0(x) \, dx = \int_{-1}^{1} (1 - x)^\alpha(1 + x)^\beta \, dx.\]  

(4.3.28)

Using the substitution \(x = 2t - 1\) this can be transformed into the equivalent integral

\[\int_{0}^{1} (2 - 2t)^\alpha(2t)^\beta \, dt = 2^{\alpha+\beta+1}\int_{0}^{1} (1 - t)^\alpha t^\beta \, dt.\]  

(4.3.29)

The integral on the right hand side of this last expression is just the beta function \(B(\alpha + 1, \beta + 1)\) and, by applying the result,

\[B(n, m) = \frac{\Gamma(n)\Gamma(m)}{\Gamma(n + m)},\]  

(4.3.30)
it is a simple matter to obtain the required form for \( N_0 \). A similar procedure can be applied to the second integral

\[
N_1 = \int_{-1}^{1} (1-x)^\alpha (1+x)^\beta T_1(x) \, dx = \int_{-1}^{1} (1-x)^\alpha (1+x)^\beta x \, dx.
\] (4.3.31)

In this case the transformation \( x = 2t - 1 \) gives

\[
\int_{0}^{1} (2 - 2t)^\alpha (2t)^\beta 2(2t - 1) \, dt = 2^{\alpha+\beta+2} \int_{-1}^{1} (1-t)^\alpha t^{\beta+1} \, dt
- 2^{\alpha+\beta+1} \int_{-1}^{1} (1-t)^\alpha t^\beta \, dt, \tag{4.3.32}
\]

where the integrals on the right hand side are equal to \( B(\alpha + 1, \beta + 2) \) and \( B(\alpha + 1, \beta + 1) \) respectively. Hence,

\[
N_1 = 2^{\alpha+\beta+1} \left[ 2B(\alpha + 1, \beta + 2) - B(\alpha + 1, \beta + 1) \right] \tag{4.3.33}
= 2^{\alpha+\beta+1} \left[ \frac{2\Gamma(\alpha + 1)\Gamma(\beta + 2)}{\Gamma(\alpha + \beta + 3)} - \frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)} \right] \tag{4.3.34}
= 2^{\alpha+\beta+1} \left[ \frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 3)} \left[ 2(\beta + 1) - (\alpha + \beta + 2) \right] \right] \tag{4.3.35}
= \frac{2^{\alpha+\beta+1}(\beta - \alpha)\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 3)}, \tag{4.3.36}
\]

which is the required result.

Using the above recurrence relation, with the starting values \( N_0 \) and \( N_1 \), it is straightforward to compute the coefficients \( R_{j,k} \) for any combination of \( j \) and \( k \). In terms of numerical stability, it is a simple exercise to show that the recurrence is stable in both the forward and backward directions.

In a numerical algorithm the Neumann series expansion must, of course, be truncated after a suitable number of terms. If a relative accuracy of \( \epsilon \) is required, the usual policy is to continue the summation until

\[
|S_{m+1} - S_m| \leq \epsilon |S_{m+1}|, \tag{4.3.37}
\]

where

\[
S_m = 2 \sum_{j=0}^{m} \hat{v} J_j(\tau) R_{j,k}, \tag{4.3.38}
\]
i.e. until the term $J_{m+1}(\tau)R_{m+1,k}$ makes no significant contribution. As the Bessel functions fall off extremely rapidly for $j > \tau$, as is evident from the asymptotic form

$$J_j(\tau) \sim \frac{1}{\sqrt{2\pi j}} \left( \frac{e\tau}{2j} \right)^j \quad j \to \infty,$$

(4.3.39)

taking $m$ to be a little larger than $\tau$ is usually sufficient. In practice it is best to over estimate this point, as this ensures that the Bessel functions, which are generated by backward recurrence for $j > \tau$, only have to be computed once.

An effective technique for computing Bessel functions of integer order, using a judicious choice of starting point for the backward recurrence, is given in [14].

Although in principle the Neumann series may be used for any value of $\tau$, it is clear that as $\tau$ increases the computational effort required to achieve a given accuracy also increases. For $\tau$ less than a thousand or so, the performance is perfectly satisfactory, however when $\tau$ rises above this level the increased workload becomes more apparent. For extreme frequencies, say $\tau \geq 10000$, the application of the expansion is not really a viable proposition. This is, of course, the drawback of the original Piessens and Poleunis method for non-singular Fourier integrals. Nevertheless, within an appropriate range, for example $\tau$ less than a thousand, this approach proves to be extremely effective, although for frequencies above this level an alternative approach is required.

To this end a second approach effective for large values of $\tau$ is introduced. The method depends upon the following asymptotic expansion due to Erdélyi [18]. Let $g(x)$ be analytic on $[-1,1]$ and define the functions

$$\theta(x) = (1 - x)^\alpha g(x), \quad \phi(x) = (1 + x)^\theta g(x).$$

(4.3.40)

Then, for $\tau > 0$

$$\int_{-1}^{1} e^{i\tau x}(1 - x)^\alpha(1 + x)^\theta g(x) = A(\tau) + B(\tau),$$

(4.3.41)

where

$$A(\tau) \sim A_P(\tau), \quad B(\tau) \sim B_P(\tau),$$

(4.3.42)
to P terms as \( r \to \infty \); with

\[
A_P(r) = -e^{ir-ir\alpha/2} \sum_{m=0}^{P-1} \frac{\phi^{(m)}(1)x^{m+1}\Gamma(m + \alpha + 1)}{\tau^{m+\alpha+1}\Gamma(m + 1)},
\]

\[
B_P(r) = e^{-ir+ir\beta/2} \sum_{m=0}^{P-1} \frac{\theta^{(m)}(-1)x^{m+1}\Gamma(m + \beta + 1)}{\tau^{m+\beta+1}\Gamma(m + 1)}.
\]

For the integrals \( \mathcal{M}_k(\alpha, \beta, \tau) \), the functions \( \theta(x) \) and \( \phi(x) \) are given by

\[
\theta(x) = (1 - x)^\alpha T_k(x), \quad \phi(x) = (1 + x)^\beta T_k(x),
\]

and their successive derivatives may be computed using the following result:

**Lemma 4.2** If \( p(x) \) is a function of the form

\[
p(x) = (1 \pm x)^{\rho} \sum_{j=0}^{k} b_{j,0} T_j(x),
\]

then

\[
\frac{d^m p(x)}{dx^m} = (1 \pm x)^{\rho-m} \sum_{j=0}^{k} b_{j,m} T_j(x),
\]

where the coefficients \( b_{j,m} \) are related to \( b_{j,m-1} \) by

\[
b_{k,m} = \pm(k + \rho + 1 - m)b_{k,m-1}
\]

\[
b_{k-1,m} = \pm(k - m + \rho)b_{k-1,m-1} + 2kb_{k,m-1}
\]

\[
b_{j-1,m} = \pm(j - m + \rho)b_{j-1,m-1} \pm (j + m - \rho)b_{j+1,m-1}
\]

\[+ 2jb_{j,m-1} + b_{j+1,m}, \quad j = k - 2, \ldots, 2
\]

\[
b_{0,m} = \pm(\rho - m + 1)b_{0,m-1} \pm (m + 1 - \rho)b_{2,m-1}/2
\]

\[+ b_{1,m-1} + b_{2,m}/2.
\]

**Proof.** It is sufficient to show that the above relations hold for the case \( m = 1 \), as the remaining part of the proof follows from a simple inductive step. Hence, differentiating \( p(x) \) gives

\[
p'(x) = (1 \pm x)^{\rho} \sum_{j=0}^{k} b_{j,0} T'_j(x) \pm \rho(1 \pm x)^{\rho-1} \sum_{j=0}^{k} b_{j,0} T_j(x)
\]

\[
= (1 \pm x)^{\rho-1} \left[(1 \pm x) \sum_{j=0}^{k} b_{j,0} T'_j(x) \pm \rho \sum_{j=0}^{k} b_{j,0} T_j(x) \right]
\]

\[
= (1 \pm x)^{\rho-1} q(x),
\]
where

\[ q(x) = (1 \pm x) \sum_{j=0}^{k} b_{j,0} T_j(x) \pm \rho \sum_{j=0}^{k} b_{j,0} T_j(x). \]  

(4.3.53)

It is clear that \( q(x) \) is a polynomial of degree \( k \) and so may be expressed in the form

\[ q(x) = \sum_{j=0}^{k} b_{j,1} T_j(x), \]  

(4.3.54)

for suitable coefficients \( \{b_{j,1}\}_{j=0}^{k} \). Equating (4.3.53) and (4.3.54) gives

\[ \sum_{j=0}^{k} b_{j,1} T_j(x) = (1 \pm x) \sum_{j=1}^{k} b_{j,0} T_j(x) \pm \rho \sum_{j=0}^{k} b_{j,0} T_j(x), \]  

(4.3.55)

where the term involving \( T_0(x) \) has been removed from the first summation on the right hand side. Integrating both sides of this last expression, and using the relation,

\[ \int T_j(x) \, dx = \frac{1}{2} \left[ \frac{T_{j+1}(x) - T_{j-1}(x)}{j} \right], \quad j \geq 2, \]  

(4.3.56)

the following formula is obtained

\[ \frac{1}{2} \sum_{j=0}^{k} b_{j,1} \left[ \frac{T_{j+1}(x)}{j+1} - \frac{T_{j-1}(x)}{j-1} \right] = \sum_{j=1}^{k} b_{j,0} T_j(x) \]  

\[ \pm \sum_{j=1}^{k} b_{j,0} \int x T_j(x) \, dx \pm \frac{\rho}{2} \sum_{j=0}^{k} b_{j,0} \left[ \frac{T_{j+1}(x)}{j+1} - \frac{T_{j-1}(x)}{j-1} \right], \]  

(4.3.57)

where it is implicitly assumed that, for \( j = 0 \) and \( j = 1 \), the integrals of the Chebyshev polynomials, and hence the bracketed terms, are given by

\[ \int T_0(x) \, dx = T_1(x), \quad \int T_1(x) \, dx = \frac{1}{4} T_2(x). \]  

(4.3.58)

Integrating the remaining integral by parts,

\[ \int x T_j(x) \, dx = x T_j(x) - \int T_j(x) \, dx \]  

\[ = \frac{1}{2} [T_{j+1}(x) + T_{j-1}(x)] - \frac{1}{2} \left[ \frac{T_{j+1}(x)}{j+1} - \frac{T_{j-1}(x)}{j-1} \right], \]  

(4.3.59)

and rearranging the terms of (4.3.57), gives

\[ \sum_{j=2}^{k} b_{j,1} \left[ \frac{T_{j+1}(x)}{j+1} - \frac{T_{j-1}(x)}{j-1} \right] + \frac{1}{2} b_{1,1} T_2(x) + 2 b_{0,1} T_1(x) = 2 \sum_{j=1}^{k} b_{j,0} T_j(x) \]  

\[ \pm \sum_{j=2}^{k} b_{j,0} \left[ T_{j+1}(x) \frac{j+\rho}{j+1} + T_{j-1}(x) \frac{j-\rho}{j-1} \right] \pm \left( \frac{1+\rho}{2} \right) b_{1,0} T_2(x) \pm 2 \rho b_{0,0} T_1(x). \]  

(4.3.60)
Equating coefficients of $T_j(x)$ on both sides, the following formulas are obtained

\begin{align*}
  b_{k,1} &= \pm (k + \rho) b_{k,0} \\
  b_{k-1,1} &= \pm (k - 1 + \rho) b_{k-1,0} + 2k b_{k,0} \\
  b_{j-1,1} &= \pm (j - 1 + \rho) b_{j-1,0} \pm (j + 1 - \rho) b_{j+1,0} \\
  &\quad + 2j b_{j,0} + b_{j+1,1}, \quad j = k - 2, \ldots, 2 \\
  b_{0,1} &= \pm \rho b_{0,0} \pm (2 - \rho) b_{2,0}/2 + b_{1,0} + b_{2,1}/2,
\end{align*}

which is precisely the result required for the particular case $m = 1$.

Using the above recurrence the derivatives of $\theta(x)$ and $\phi(x)$ can be found in the following way: set $\rho = \alpha$ and $\rho = \beta$ respectively, and apply the relations (4.3.48)-(4.3.51) recursively for $m = 1, 2, \ldots$, using the starting values $b_{k,0} = 1$ and $b_{j,0} = 0$ for $j = k - 1, \ldots, 0$.

In practice, the asymptotic expansion can only be used to accurately evaluate the integrals $M_k(\alpha, \beta, \tau)$ provided $\tau$ is sufficiently large in comparison to $k$. The reason for this is best seen by examining how the magnitudes of $\phi^{(m)}(1)$ and $\theta^{(m)}(-1)$ vary as $k$ increases. Using Leibnitz's theorem,

\begin{align*}
  \phi^{(m)}(1) &= \sum_{j=0}^{m} \binom{m}{j} \frac{d^{m-j}}{dx^{m-j}} (1 + x)^{\beta} \left. \frac{d^j}{dx^j} T_k(x) \right|_{x=1} \\
  \theta^{(m)}(-1) &= \sum_{j=0}^{m} \binom{m}{j} \frac{d^{m-j}}{dx^{m-j}} (1 - x)^{\alpha} \left. \frac{d^j}{dx^j} T_k(x) \right|_{x=-1},
\end{align*}

where $|_{x=\pm1}$ denotes evaluation at $x = \pm1$. For $j \geq 1$, the derivatives of the Chebyshev polynomials are given by

\begin{equation}
  (\pm1)^j \frac{k^2(k^2 - 1^2)(k^2 - 2^2) \cdots (k^2 - (j-1)^2)}{1.3.5 \cdots (2j-1)},
\end{equation}

and hence the derivatives grow rapidly in magnitude as $k$ increases. From (4.3.65) and (4.3.66) it follows that as $k$ increases the magnitudes of the derivatives of $\phi^{(m)}(x)$ and $\theta^{(m)}(x)$ increase at a correspondingly rapid rate. As a consequence of this, if $\tau$ is too small in comparison to $k$, the terms of the asymptotic expansion increase in size so quickly that there is little chance in using the expansion to
evaluate the required integrals accurately. However, if \( \tau \) is sufficiently large relative to \( k \), the initial terms of the expansion decrease rapidly, giving the numerical appearance of a convergent series, and accurate values can be obtained for the required integrals. Exact conditions are difficult to formulate, but as a rough guide, accurate values for the integrals \( M_k(\alpha, \beta, \tau) \) correct to 15 significant figures can be obtained provided \( \tau \) is larger than \( k^{3/2} \). In fact, for moderate values of \( k \), say \( k \leq 50 \), this is a gross over-estimate and the relationship is closer to \( \tau > 3k/2 \). For example, if \( \tau \geq 50 \), the integrals \( M_k(\alpha, \beta, \tau) \) may be computed accurately using the asymptotic expansion for all \( k \) up to and including \( k = 32 \).

Of course, for such small values of \( \tau \) the Neumann series expansion is very effective, and the suggestion is to use that approach for values of \( \tau \) up to a thousand or so, and then switch to the asymptotic expansion above this level. For example, if the switch-over point is set as \( \tau = 500 \), the asymptotic expansion can be used to accurately compute the necessary integrals for all \( k \) up to and including \( k = 64 \). As most smooth functions can be accurately approximated by a Chebyshev expansion whose order is much less than 64, this would seem a sensible switch-over point. For more extreme examples, in which the non-singular, non-oscillatory part of the integrand exhibits some other peculiar behaviour, it may be necessary to employ higher order approximations, in which case the suggestion is to set the switch-over point to \( \tau = 1000 \). In this case the asymptotic expansion is valid for \( k \leq 128 \).

### 4.4 Extensions to logarithmic singularities

In this section it is shown how the methods developed for algebraic singularities can be extended to deal with the integral

\[
M_k(\alpha, \beta, 1, 1, \tau) = \int_{-1}^{1} e^{i\tau x} \ln(1 - x)(1 - x)^{\alpha}(1 + x)^{\beta} \ln(1 + x)T_k(x) \, dx. \tag{4.4.1}
\]

The cases where a logarithmic singularity occurs at only one end-point can be interpreted as particular instances of the following formulas.

From Section 4.3, it is clear that to extend the Neumann series approach to
CHAPTER 4. SINGULAR OSCILLATORY INTEGRALS

the integral (4.4.1), all that is required is a routine for computing the integrals

$$\int_{-1}^{1} \ln(1-x)(1-x)^{\alpha}(1+x)^{\beta} \ln(1+x)T_{n}(x)dx.$$  \hspace{1cm} (4.4.2)

If $N_{n}$ denotes the integral

$$\int_{-1}^{1} (1-x)^{\alpha}(1+x)^{\beta}T_{n}(x)dx,$$  \hspace{1cm} (4.4.3)

then

$$N_{n}(\alpha) = \frac{\partial N_{n}}{\partial \alpha} = \int_{-1}^{1} \ln(1-x)(1-x)^{\alpha}(1+x)^{\beta}T_{n}(x)dx,$$  \hspace{1cm} (4.4.4)

$$N_{n}(\beta) = \frac{\partial N_{n}}{\partial \beta} = \int_{-1}^{1} (1-x)^{\alpha}(1+x)^{\beta} \ln(1+x)T_{n}(x)dx,$$  \hspace{1cm} (4.4.5)

and

$$N_{n}(\alpha, \beta) = \frac{\partial^2 N_{n}}{\partial \alpha \partial \beta} = \int_{-1}^{1} (1-x)^{\alpha} \ln(1-x)(1+x)^{\beta} \ln(1+x)T_{n}(x)dx.$$  \hspace{1cm} (4.4.6)

Hence, by differentiating the recurrence relation satisfied by $N_{n}$ with respect to $\alpha$ and $\beta$, it is a simple exercise to show that if $z_{n}$ denotes either $N_{n}(\alpha)$, $N_{n}(\beta)$ or $N_{n}(\alpha, \beta)$, then

$$(n/2 + 1 + \alpha/2 + \beta/2)z_{n+1} - (\beta - \alpha)z_{n} - (n/2 - 1 - \alpha/2 - \beta/2)z_{n-1} = y_{n},$$  \hspace{1cm} (4.4.7)

where $y_{n}$ is given by

$$y_{n} = -N_{n} - \frac{1}{2}(N_{n+1} + N_{n-1}),$$  \hspace{1cm} (4.4.8)

$$y_{n} = N_{n} - \frac{1}{2}(N_{n+1} + N_{n-1}),$$  \hspace{1cm} (4.4.9)

and

$$y_{n} = N_{n}^{\alpha} - N_{n}^{\beta} - \frac{1}{2}(N_{n+1}^{\alpha} + N_{n-1}^{\alpha}) - \frac{1}{2}(N_{n+1}^{\beta} + N_{n-1}^{\beta}),$$  \hspace{1cm} (4.4.10)

for the three respective cases.

Using the above recurrence relations it is straightforward to compute the integral $N_{n}(\alpha, \beta)$ for any given value of $n$. The starting values necessary to begin each recurrence may be obtained by differentiating equations (4.3.11) and (4.3.12) with respect to $\alpha$ and $\beta$ as appropriate. It should be noted, however, that the
resulting formulas are more complicated than those given previously, and involve
the Digamma function $\Psi(z)$, defined by $\Psi(z) = \Gamma'(z)/\Gamma(z)$. For example,

$$
N_0^\alpha = \left[ \ln 2 + \Psi(\alpha + 1) - \Psi(\alpha + \beta + 2) \right] \\
\times \frac{2^{\alpha+\beta+1} \Gamma(\alpha + 1) \Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)}, 
$$

(4.4.11)

$$
N_1^\alpha = \left[ \ln 2 - \Psi(\alpha + 1) + \Psi(\alpha + \beta + 3) \right] \\
\times \frac{2^{\alpha+\beta+1} (\beta - \alpha) \Gamma(\alpha + 1) \Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 3)}, 
$$

(4.4.12)

with similar expressions for the other initial values.

The extension of the asymptotic method relies on the following asymptotic
expansion due to Lyness [49]. Let $h(x)$ be analytic on $[-1,1]$ and define the functions

$$
\theta(x) = \ln(1-x)(1-x)^\alpha h(x), \quad \phi(x) = \ln(1+x)(1+x)^\beta h(x). 
$$

(4.4.13)

Then, for $\tau > 0$

$$
\int_{-1}^{1} e^{ix\tau} \ln(1-x)(1-x)^\alpha(1+x)^\beta \ln(1+x)h(x) = A(\tau) + B(\tau), 
$$

(4.4.14)

where

$$
A(\tau) \sim A_P(\tau), \quad B(\tau) \sim B_P(\tau), 
$$

(4.4.15)

to $P$ terms as $\tau \to \infty$; with

$$
A_P(\tau) = -e^{i\tau - i\pi \alpha/2} \sum_{m=0}^{P-1} \frac{\theta^m(1) \tau^{m+1} \Gamma(m + \alpha + 1)}{\tau^{m+\alpha+1} \Gamma(m + 1)} \\
\times [\Psi(m + \alpha + 1) - \ln(\tau) - i\pi/2], 
$$

(4.4.16)

$$
B_P(\tau) = e^{-i\tau + i\pi \beta/2} \sum_{m=0}^{P-1} \frac{\theta^m(-1) \tau^{m+1} \Gamma(m + \beta + 1)}{\tau^{m+\beta+1} \Gamma(m + 1)} \\
\times [\Psi(m + \beta + 1) - \ln(\tau) + i\pi/2]. 
$$

(4.4.17)

For the integral (4.4.1) the functions $\theta(x)$ and $\phi(x)$ are given by

$$
\theta(x) = \ln(1-x)(1-x)^\alpha T_k(x), 
$$

(4.4.18)
and

\[ \phi(x) = \ln(1 + x)(1 + x)\beta T_k(x), \quad (4.4.19) \]

and their derivatives follow in a manner similar to the previous section. Hence, if

\[ p(x) = \ln(1 \pm x)(1 \pm x)\rho \sum_{j=0}^{k} b_j T_j(x) + (1 \pm x)\rho \sum_{j=0}^{k} c_{j,0} T_j(x), \quad (4.4.20) \]

then

\[
\frac{d^m p(x)}{dx^m} = \ln(1 \pm x)(1 \pm x)\rho - m \sum_{j=0}^{k} b_{j,m} T_k(x) \\
+ (1 \pm x)\rho - m \sum_{j=0}^{k} c_{j,m} T_j(x). \quad (4.4.21)
\]

The coefficients \( \{b_{j,m}\}_{j=0}^{k} \) can be determined from the coefficient \( \{b_{j,m-1}\}_{j=0}^{k} \) using the recurrence relations (4.3.48)-(4.3.51). The coefficients \( \{c_{j,m}\}_{j=0}^{k} \) can also be found in this manner, provided the right hand side of each equation is adjusted to contain the additional term \( \pm b_{j,m-1} \). The derivatives of \( \theta(x) \) and \( \phi(x) \) can then be computed by setting \( \rho = \alpha \) and \( \rho = \beta \) respectively, and applying the recurrence for \( m = 0, 1, \ldots \), with the starting values \( b_{k,0} = 1, c_{k,0} = 0, \) and \( b_{j,0} = c_{j,0} = 0 \) for \( j = k - 1, \ldots, 0 \).

As in the purely algebraic case the suggestion is to use the Neumann series to evaluate the integrals \( M_k(\alpha, \beta, r, s, \tau) \) for values of \( \tau \leq 500 \), and then switch to the asymptotic expansion for values of \( \tau \) above this point.

### 4.5 Practical implementation and numerical examples

Before moving on to discuss the practical implementation of the proposed method, it is useful to highlight some results which apply to extended Clenshaw-Curtis integration rules in general, and hence are relevant to the method presented here.

From a theoretical perspective, the results of Sloan and Smith [71] discussed previously, establish a sound basis for the method. In addition, their results also
have practical implications, as they provide a guarantee of numerical stability when $n$ is large, in the sense that the amplification of roundoff errors and the effects of subtractive cancellation are minimised. From a computational standpoint, probably the most important aspect is the estimation of the truncation error in the integration rule. Error bounds for the truncation error, which are, on the whole, reliable and accurate, have been obtained by Sloan and Smith [72] and Adam and Nobile [2], and any of these estimates may be used in a routine employing the proposed algorithm. As a final practical point, if the evaluation of the coefficients $a_0, \ldots, a_n$ is dominated by the calculation of $(n + 1)^2$ cosines, rather than $n + 1$ evaluations of $f(x)$, then the fast cosine transform [19] should be used to evaluate the expression (4.2.4).

The actual implementation of the proposed algorithm is not especially difficult, but some care has to be taken to avoid introducing unnecessary errors into the calculation. For the Neumann series, the prime concern is to compute the Bessel functions efficiently and accurately, and an effective way to do this is presented in [14]. The algorithm is based on the usual device of using the recurrence relation

$$J_{k+1}(x) + J_{k-1}(x) = \frac{2k}{x}J_k(x), \quad (4.5.1)$$

in the reverse direction for $k > x$, but the method appears to be better than many alternative algorithms, because the starting point for the backward recurrence is determined using more precise criteria.

The calculation of the coefficients $R_{j,k}$, and hence the integrals $N_n$, is also a concern. Although the recurrence is numerically stable in the forward direction, the accurate evaluation of $N_n$ for $n \geq 2$ is still dependent on obtaining accurate values for the initial terms $N_0$ and $N_1$. This, in turn, requires an accurate routine to evaluate the Gamma function, $\Gamma(x)$, in the case of algebraic singularities, and the Digamma function, $\Psi(x)$, in the case of logarithmic singularities. To evaluate $\Gamma(x)$ a common technique is to use Stirling's asymptotic approximation for large
arguments, and for small arguments repeatedly apply the relation

$$\Gamma(x) = \frac{\Gamma(x + 1)}{x}, \quad (4.5.2)$$

to increase the argument to a point where Stirling’s approximation can be applied. In most cases this is a satisfactory approach, however for $x$ near to zero (say $x < 0.1$), this procedure leads to a loss of significance in the calculation. A better method is to use the series expansion

$$\Gamma(x) = \frac{1}{x} - \gamma + \left(\frac{1}{12}x^2 + \frac{1}{2!}x^2\right) x + \cdots, \quad (4.5.3)$$

for small arguments $x$. This remark is relevant for very singular integrals where $\alpha$ and $\beta$ are close to $-1$, as in this case the Gamma functions $\Gamma(\alpha + 1)$ and $\Gamma(\beta + 1)$ in the initial values $N_0$ and $N_1$ are required for arguments close to zero. Similar care should be taken with the evaluation of the Digamma function for small values of $x$.

The remarks regarding the evaluation of the Gamma and Digamma functions are also relevant for the asymptotic expansions. It should also be noted, that by arranging the computation appropriately, the number of arithmetic operations required to evaluate each asymptotic series may be reduced significantly. For example, in the case of algebraic singularities, each term of the asymptotic expansion contains a quotient of the form

$$p_m = \frac{\Gamma(m + \rho + 1)}{\tau^{m+\rho+1} \Gamma(m + 1)}$$

$$= \frac{m + \rho}{m\tau} \left[ \frac{\Gamma(m + \rho)}{\tau^{m+\rho} \Gamma(m)} \right]$$

$$= \frac{m + \rho}{m\tau} p_{m-1}, \quad (4.5.4)$$

and hence $p_m$ may be determined from $p_{m-1}$ by multiplying by $(m + \rho)/m\tau$. As a consequence, it is only necessary to evaluate the Gamma functions in the first term of each part of the asymptotic expansion, as the remaining terms can be evaluated using the simple recurrence given above. Hence, only $\Gamma(\alpha + 1)$ and $\Gamma(\beta + 1)$ are
required. This device also avoids potential overflow when computing the Gamma function for large arguments. Similar remarks hold for the logarithmic asymptotic expansion.

If the singular oscillatory integral is evaluated for two or more values of $\tau$, then a further saving may be made by storing the values of the individual terms of the asymptotic series at the first evaluation. Then, to evaluate the asymptotic series for $\tau = \tau_2$, where the terms for $\tau = \tau_1$ have been computed and stored, it is only necessary to multiply each term by $(\tau_1/\tau_2)^{m+p+1}$ ($\rho = \alpha$ or $\rho = \beta$) for $m = 0, 1, \ldots$, and then re-sum the series.

A final practical point concerns the evaluation of the derivatives of $\theta(x)$ and $\phi(x)$. If a selection of integrals is computed for a range of frequencies, then it is best to compute the derivatives for $k = 1, \ldots, n$ and $m = 0, 1, \ldots$, where $n$ is the maximum order used, and store the values for later use. However, if only a single integral is evaluated for a range of frequencies, then for the algebraic case it is more efficient to take the function $\theta(x)$ and $\phi(x)$ to be

$$\theta(x) = (1 - x)^{\alpha} \sum_{k=0}^{n} a_k T_k(x),$$

$$\phi(x) = (1 + x)^{\delta} \sum_{k=0}^{n} a_k T_k(x),$$

as this avoids having to repeatedly apply equations (4.3.48)-(4.3.51) for each value of $k$. Similarly, for logarithmic singularities, the functions $\theta(x)$ and $\phi(x)$ should be taken as

$$\theta(x) = \ln(1 - x)(1 - x)^{\alpha} \sum_{k=0}^{n} a_k T_k(x),$$

$$\phi(x) = \ln(1 + x)(1 + x)^{\delta} \sum_{k=0}^{n} a_k T_k(x).$$

To demonstrate the effectiveness of the proposed method, a selection of singular oscillatory integrals have been evaluated for a range of $\tau$, $\alpha$ and $\beta$. For each example an analytic integral is given and this was used to confirm the accuracy of the results presented below. The computations were carried out in double precision arithmetic (approximately 15 significant figures).
Example 1 The integral

\[ I_1(a, \tau) = \int_0^1 \frac{\sin(ax)}{x^{1/2}} \cos(\tau x) \, dx, \quad a, \tau > 0, \tag{4.5.9} \]

has been evaluated for various combinations of \(a\) and \(\tau\). The exact value is

\[
I_1(a, \tau) = \frac{\sqrt{\pi}}{\sqrt{2\sqrt{\pi} + a}} S \left( \frac{\sqrt{2\sqrt{\tau + a}}}{\sqrt{\pi}} \right) \\
\pm \frac{\sqrt{\pi}}{\sqrt{2\sqrt{|a - \tau|}} S \left( \frac{\sqrt{2\sqrt{|a - \tau|}}}{\sqrt{\pi}} \right)}, \quad \tau \neq a, \tag{4.5.10}
\]

where \(S(x)\) is the Fresnel Sine integral. The sign in (4.5.10) is taken as plus if \(\tau < a\) and minus if \(\tau > a\). The relative errors achieved for various values of \(n\) are presented in Table 4.1. As a comparison, for the particular case \(\tau = 500, a = 35\pi/4\), the extended Clenshaw-Curtis method described in [28], which only takes into account the oscillatory part of the integrand, requires well in excess of 300 function evaluations to achieve a relative error comparable to the present method for \(n = 37\).

Example 2 The integral

\[ I_2(\nu, \tau) = \int_0^1 x(1 - x^2)^\nu \cos(\tau x) \, dx, \quad \tau > 0, \quad \nu > -1, \tag{4.5.11} \]

has been evaluated for various combinations of \(\nu\) and \(\tau\). The exact value is

\[
I_2(\nu, \tau) = \frac{1}{2} (\nu + 1)^{-1} - \frac{\sqrt{\pi}}{2} \left( \frac{2}{\tau} \right)^{\nu+1/2} \Gamma(\nu + 1) \text{H}_{\nu+3/2}(\tau), \tag{4.5.12}
\]

where \(\text{H}_\nu(z)\) is Struve's function (Abramowitz and Stegun [1], p.496). The results are given in Table 4.2. This example illustrates the ability of the proposed method to cope with increasingly severe singular behaviour, especially in the extreme case \(\nu = -999/1000\), which is barely distinguishable from the divergent example \(\nu = -1\).

Example 3 The final integral considered was

\[ I_3(\lambda, n, \tau) = \int_{-1}^{1} (1 - x^2)^{\lambda-1/2} C_n^\lambda(x) \cos(\tau x) \, dx, \quad \lambda > -1/2, \tag{4.5.13} \]
where \( C_n^\lambda(x) \) is the Gegenbauer polynomial of degree \( n \). The exact value is given by

\[
I_3(\lambda, n, \tau) = \left( \frac{2}{\pi} \right)^\lambda J_{n+\lambda}(\tau) \frac{\pi^{21-2\lambda} \Gamma(n + 2\lambda)}{n! \Gamma(n + \lambda)}, \quad \text{even},
\]

where the integrals for odd \( n \) vanish by symmetry. This example is unusual, in that the function to be approximated can be fitted exactly using a Chebyshev series of degree \( n \). Consequently, any errors in the computed values of (4.5.13) may be attributed to errors in the computation of the fundamental integrals

\[
M_k(\rho, \tau) = \int_{-1}^{1} (1 - x^2)^\rho T_k(x) \cos(\tau x) \, dx, \quad \rho = \lambda - 1/2, \lambda > -1/2. \tag{4.5.15}
\]

This example is therefore a good test of the proposed method's ability to compute high accuracy values for (4.5.15). Results for \( I_3(1/3, n, \tau) \), with various combinations of \( n \) and \( \tau \), are presented in Table 4.3.

Clearly, the accuracy achieved in evaluating the integrals (4.5.15) is reflected in the results obtained for \( I_3(1/3, n, \tau) \). Even when these integrals are required for \( k \) as high as 96, there is no apparent loss in accuracy.

†Computed using Neumann series.

‡Computed using asymptotic expansion.
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<th>$n$</th>
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<td>$5^t$</td>
<td>$35\pi/4$</td>
<td>$2.5427526561802(-1)$</td>
<td></td>
<td>1.9(-4)</td>
<td>6.7(-10)</td>
<td>3.8(-14)</td>
</tr>
<tr>
<td>$50^t$</td>
<td>$35\pi/4$</td>
<td>$-7.7212343020380(-2)$</td>
<td></td>
<td>3.4(-2)</td>
<td>4.0(-5)</td>
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<tr>
<td>$500^t$</td>
<td>$35\pi/4$</td>
<td>$-2.1369409113647(-3)$</td>
<td></td>
<td>2.5(-1)</td>
<td>7.8(-6)</td>
<td>6.2(-12)</td>
</tr>
<tr>
<td>$5000^t$</td>
<td>$35\pi/4$</td>
<td>$-1.8856985606749(-4)$</td>
<td></td>
<td>1.6(-1)</td>
<td>4.3(-6)</td>
<td>4.1(-13)</td>
</tr>
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<table>
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<tr>
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<th>$a$</th>
<th>Exact value</th>
<th>$n$</th>
<th>22</th>
<th>41</th>
<th>50</th>
</tr>
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<tbody>
<tr>
<td>$5^t$</td>
<td>$73\pi/4$</td>
<td>$1.6346061422714(-1)$</td>
<td></td>
<td>1.1(-4)</td>
<td>1.3(-9)</td>
<td>1.2(-15)</td>
</tr>
<tr>
<td>$50^t$</td>
<td>$73\pi/4$</td>
<td>$2.5057028314091(-1)$</td>
<td></td>
<td>4.5(-1)</td>
<td>1.4(-9)</td>
<td>8.7(-14)</td>
</tr>
<tr>
<td>$500^t$</td>
<td>$73\pi/4$</td>
<td>$-4.0546897010803(-3)$</td>
<td></td>
<td>1.3(-1)</td>
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<td>$5000^t$</td>
<td>$73\pi/4$</td>
<td>$-2.4111991879756(-4)$</td>
<td></td>
<td>2.5(-1)</td>
<td>1.3(-5)</td>
<td>2.0(-9)</td>
</tr>
</tbody>
</table>

Table 4.1: Relative errors in the numerical evaluation of $I_1(a, \tau)$
### Table 4.2: Order $n$ required to evaluate $I_2(\nu, \tau)$ to 14 significant figures

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>$\nu$</th>
<th>Exact value</th>
<th>$n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1^t$</td>
<td>-1/3</td>
<td>5.3868479035755(-1)</td>
<td>13</td>
</tr>
<tr>
<td>$10^t$</td>
<td>-1/3</td>
<td>-2.2214686990851(-1)</td>
<td>14</td>
</tr>
<tr>
<td>$100^t$</td>
<td>-1/3</td>
<td>-1.9031679268277(-4)</td>
<td>15</td>
</tr>
<tr>
<td>$1000^t$</td>
<td>-1/3</td>
<td>1.0717936788154(-2)</td>
<td>13</td>
</tr>
<tr>
<td>$10000^t$</td>
<td>-1/3</td>
<td>-1.7153040210575(-3)</td>
<td>13</td>
</tr>
<tr>
<td>$1^t$</td>
<td>-2/3</td>
<td>9.7649287732387(-1)</td>
<td>14</td>
</tr>
<tr>
<td>$10^t$</td>
<td>-2/3</td>
<td>-7.9170580853299(-1)</td>
<td>14</td>
</tr>
<tr>
<td>$100^t$</td>
<td>-2/3</td>
<td>1.8007386209414(-1)</td>
<td>15</td>
</tr>
<tr>
<td>$1000^t$</td>
<td>-2/3</td>
<td>1.5194905044727(-1)</td>
<td>14</td>
</tr>
<tr>
<td>$10000^t$</td>
<td>-2/3</td>
<td>-7.6562536387247(-2)</td>
<td>13</td>
</tr>
</tbody>
</table>

Table 4.2: Order $n$ required to evaluate $I_2(\nu, \tau)$ to 14 significant figures
### Table 4.3: No. of significant figures achieved in the evaluation of $I_3(1/3, n, \tau)$

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>$n$</th>
<th>Exact value</th>
<th>No. sig. figures</th>
</tr>
</thead>
<tbody>
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<td>100\dagger</td>
<td>32</td>
<td>-9.8909574535657(-3)</td>
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<td>14</td>
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<td>100\dagger</td>
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<td>6.1959210792237(-3)</td>
<td>14</td>
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<td>1000\dagger</td>
<td>64</td>
<td>-1.9125436575397(-4)</td>
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<tr>
<td>100\dagger</td>
<td>96</td>
<td>1.2780373816590(-2)</td>
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<tr>
<td>1000\dagger</td>
<td>96</td>
<td>-4.0414966015790(-4)</td>
<td>14</td>
</tr>
</tbody>
</table>
Chapter 5

Conclusions

5.1 A brief review

The evaluation of rapidly oscillatory integrals is a common requirement throughout physics and applied mathematics. The survey presented in Chapter 1 highlights the fact that many oscillatory integrals cannot be evaluated satisfactorily using existing numerical integration schemes and that there is a requirement to develop new integration methods to calculate these integrals. The methods presented here make significant progress towards solving this problem and permit the fast and accurate calculation of a wide range of oscillatory integrals.

The integration rule introduced in Chapter 2 is an effective tool for evaluating irregular trigonometric integrals. The choice of cosine-distributed abscissae results in a formula that is, in practice, convergent and numerically stable as the order $n$ is increased. The method is competitive with alternative techniques and should be considered the formula of choice for this class of integral.

An extension of this approach is considered in Chapter 3. Through the use of Lagrange's identity, a technique is derived which allows a numerical integration rule to be constructed for any oscillatory integral, provided that the oscillatory kernel satisfies a linear differential equation of $m \geq 1$. The method has been successfully used to evaluate rapidly oscillatory integrals involving Bessel functions.
of a linear and nonlinear argument.

Finally, the routine presented in Chapter 4 can be used to evaluate singular Fourier transforms, where the singularities are algebraic or logarithmic. The algorithm is robust and efficient, and can be economised significantly when the calculation is performed for a range of oscillatory frequencies.

5.2 Future development

The main areas open to further study concern the numerical integration rule introduced in Chapter 3. There are three principal questions: For a weight function \( w(x) \) and a function \( f(x) \) can the abscissae \( \{x_j\}_{j=0}^{n} \) and the functions \( \{z_k(x)\}_{k=0}^{n} \) be selected so that the method converges as \( n \to \infty \)? If they can, what are the conditions on \( w(x) \) and \( f(x) \) which guarantee convergence? And if the method converges, what is the rate of convergence?

Although these are important questions, it appears to be very difficult to obtain even partial solutions to these problems in the present case. Most results on the convergence of numerical integration rules are specific to interpolatory rules, where the formula is exact for any polynomial of degree \( \leq n \). In this case, the usual device is to rely on specific representations of the interpolating polynomial to prove or disprove convergence. For the present formula this method is not applicable, as the approximation is based on a non-standard set of functions. An alternative idea is to use the result of Krylov [38, Chap. 12], who demonstrates that the approximate integration rule \( \sum_{j=0}^{n} w_j f(x_j) \approx \int_a^b w(x) f(x) \, dx \) for a general matrix of integration weights and abscissae, converges if there exists a number \( K < \infty \) such that \( \sum_{j=0}^{n} |w_j| \leq K \) for \( n = 0, 1, 2, \ldots \) and the process converges for each polynomial. In the present case, however, the integration weights are determined from a system of linear equations, and there seems to be no obvious way to estimate the above limit for the general case.
Appendix A

Addendum

A.1 Recurrence relations for algebraic and logarithmic integrals

Chapter 4 introduces a method for the evaluation of oscillatory integrals in which the non-oscillatory part of the integrand possesses algebraic and logarithmic singularities at the end-points of integration. Specifically, integrals of the form

\[ \int_a^b e^{ix} h(x) g(x) \, dx, \quad -\infty < a < b < \infty, \]  

are considered, where \( h(x) \) has the form

\[ h(x) = [\ln(b-x)]^r [b-x]^\beta [\ln(x-a)]^s, \quad r, s = 0, 1, \]  

with \( \alpha, \beta > -1 \) and \( g(x) \) is supposed non-oscillatory.

Using a linear transformation to convert the interval of integration from \([a, b]\) to \([-1, 1]\) the evaluation of such integrals is reduced to the evaluation of a series of integrals of the form

\[ M_k(\alpha, \beta, r, s, \tau) = \int_{-1}^1 e^{ix} [\ln(1-x)]^r (1-x)^\alpha (1+x)^\beta [\ln(1+x)]^s T_k(x) \, dx. \]  

The evaluation of (A.1.3) is performed using a Neumann series expansion if the oscillatory frequency is less than 1000, or an asymptotic expansion otherwise.
In the case of the Neumann series approach, the computation makes use of
the recurrence relation (4.3.10) derived in Lemma 4.1. The derivation of this
recurrence relation has, in fact, appeared in prior form in Smith [73]. Smith’s
motivation is the numerical evaluation of a class of divergent integrals
\[ \int_0^1 x^\alpha (1-x)^\beta f(x) \, dx, \]  
(A.1.4)
in which both \( \alpha \) and \( \beta \) are real and non-integral and either \( \alpha < -1 \) or \( \beta < -1 \) or
both. Smith’s approach is to approximate the function \( f \), which is assumed to be
regular in the interval \([0, 1]\), using a series of shifted Chebyshev polynomials
\[ T_n^*(x) = T_n(2x - 1), \]  
(A.1.5)
where \( T_n(x) \) is the Chebyshev polynomial of degree \( n \) in \( x \). The evaluation of
(A.1.4) then reduces to the computation of
\[ M_n^* = \int_0^1 x^\alpha (1-t)^\beta T_n^*(x) \, dx, \]  
(A.1.6)
where \( M_n^* \) is a function of \( \alpha \) and \( \beta \). The integrals (A.1.6) can be rewritten as
\[ M_n^* = 2^{-(\alpha + \beta + 1)} \int_{-1}^1 (1+x)^\alpha (1-x)^\beta T_n(x) \, dx, \]  
(A.1.7)
which aside from the constant factor is equivalent to the integrals \( N_n \) defined in
equation (4.3.7). Smith’s derivation of the recurrence relation for (A.1.6) then
proceeds along similar lines to the derivation presented in Lemma 4.1.

Although the recurrence relation makes the two methods appear similar at
first sight, there are significant differences between Smith’s method and the present
approach. In Smith’s method the recurrence relation is a key aspect of the inte­
gregation rule, whereas in the present method the recurrence is of secondary impor­
tance. Of principal importance is the fact that provided the auxiliary integrals
\[ \int_{-1}^1 e^{ix} H(x) T_k(x) \, dx, \quad k = 0, 1, 2, \ldots, \]  
(A.1.8)
can be evaluated efficiently, where
\[ H(x) = h(t), \quad t = \frac{1}{2}(b-a)x + \frac{1}{2}(b+a), \]  
(A.1.9)
then it is possible to use a Neumann series expansion to evaluate the integral
\[ \int_{a}^{b} e^{i\tau x} h(x) g(x) \, dx, \quad -\infty < a < b < \infty, \]  
(A.1.10)
by using the relation (4.3.2) and expanding \( g(x) \) as a finite series of Chebyshev polynomials. The method developed in Chapter 4 is therefore not only appropriate for singular weight functions \( h(x) \) but also for a variety of other weight functions. In the singular case the evaluation of (A.1.8) is performed using the recurrence relation of Lemma 4.1, but any alternative technique would be suitable. One such technique is presented in the next section.

Additionally, in Chapter 4 it is stated without proof that the recurrence relation (4.3.10) is numerically stable in the forward and backward directions. A proof of this is also presented in Smith [73]. However, a derivation of all the relevant asymptotic expansions is not presented in that paper and so is provided here for completeness.

The numerical stability of a recurrence relation depends on the asymptotic behaviour as \( n \to \infty \) of all solutions of the difference equation. Wong and Li [84] detail a method for deriving such asymptotic expansions. For a difference equation
\[ y(n + 2) + a(n)y(n + 1) + b(n)y(n) = 0, \]  
(A.1.11)
where \( a(n) \) and \( b(n) \) have asymptotic expansions of the form
\[ a(n) \sim \sum_{k=0}^{\infty} \frac{a_k}{n^k}, \quad b(n) \sim \sum_{k=0}^{\infty} \frac{b_k}{n^k}, \]  
(A.1.12)
for large values of \( n \) and \( b_0 \neq 0 \), the asymptotic solutions are classified by the roots of the characteristic equation
\[ \rho^2 + a_0 \rho + b_0 = 0. \]  
(A.1.13)
Expressing the recurrence (4.3.10) in the form (A.1.11) it is straightforward to show that
\[ a(n) \sim \frac{2\alpha - 2\beta}{n}, \quad b(n) \sim -1 + \frac{4 + 2\alpha + 2\beta}{n}. \]  
(A.1.14)
Hence the characteristic equation is

\[ \rho^2 - 1 = 0, \tag{A.1.15} \]

which has roots \( \rho = \pm 1 \). As the roots are distinct the difference equation has two linearly independent solutions, both of the form

\[ y(n) \sim \rho^n n^\lambda \sum_{k=0}^{\infty} \frac{c_k}{n^k}, \tag{A.1.16} \]

where

\[ \lambda = \frac{a_1 \rho + b_1}{a_0 \rho + 2b_0}. \tag{A.1.17} \]

Hence, taking each root in turn, the asymptotic expansions of the solutions to one term are

\[ y_1(n) \sim \frac{c}{n^{2\alpha+2}}, \quad y_2(n) \sim \frac{d}{n^{2\beta+2}}, \tag{A.1.18} \]

where \( c \) and \( d \) are constants. Comparing the above asymptotic expansions with that of \( M_n^* \) in Smith [73, pp. 281] it follows that the recurrence relation is stable in the forward and backward directions.

A further point to highlight is the derivation of the equivalent recurrence relation (4.4.7)-(4.4.10) for logarithmic integrals. This is done by partial differentiating the original integral \( N_n \) and its' associated recurrence relation with respect to the parameters \( \alpha \) and \( \beta \). A similar technique has been used previously by Lyness and Ninham [52] to derive asymptotic expansions of integrals with algebraic and logarithmic singularities. In particular, the generalised Euler-Maclaurin expansion for integrals with logarithmic singularities is derived from that for algebraic singularities by partial differentiation with respect to the appropriate parameters. This technique is applicable in a range of situations and is often the most effective way to pass from results for algebraic singularities to the equivalent results for logarithmic singularities.

The final remark concerns the use of Erdőlyi's and Lyness' asymptotic expansions to evaluate the singular Fourier integral (A.1.1) as described in Chapter
Rather than apply the expansions directly to the original integral, the function \( g(x) \) is approximated with a finite Chebyshev series and then the asymptotic expansion is evaluated with the approximation in place of \( g(x) \). This approach has two advantages. First, it does not require the derivatives of \( g(x) \), but only the derivatives of the polynomial approximation. Second, the derivatives in the terms of the asymptotic expansions can be evaluated using the recurrence relations presented in Sections 4.3 and 4.4.

A method that is similar to this in philosophy, although not in detail, is described by Smith [74]. The technique is suitable for divergent integrals of the form

\[
\int_0^1 x^\alpha f(x) \, dx,
\]  

(A.1.19)

in which \( \alpha < -1 \) and \( 2\alpha \) is non-integral and where the function \( f \) is assumed to be regular in some region containing the interval \([0, 1]\). Smith approximates \( f \) using a finite series of shifted Chebyshev polynomials, which leaves the task of evaluating integrals of the form

\[
M_n(\alpha) = \int_0^1 x^\alpha T_n^*(x) \, dx, \quad \alpha < -1.
\]  

(A.1.20)

Interpreting this integral using generalised function theory, Smith shows that

\[
M_n(\alpha) = \frac{T_n^*(1)}{(\alpha + 1)} - \frac{T_n'(1)}{(\alpha + 1)(\alpha + 2)} + \cdots + \frac{(-1)^n T_n^{(n)}(1)}{(\alpha + 1) \cdots (\alpha + n + 1)},
\]  

(A.1.21)

and derives the following recurrence for evaluating the terms of this series

\[
u_{j+1} = \frac{-2}{(\alpha + j + 2) \left( \frac{n^2 - j^2}{2j + 1} \right)} \, u_j, \quad 0 \leq j \leq n - 1,
\]  

(A.1.22)

where

\[
u_j = \frac{(-1)^j T_n^*(j)(1)}{(\alpha + 1) \cdots (\alpha + j + 1)}.
\]  

(A.1.23)

In this form it is possible to see the common theme between the two methods. Both integration rules are based on series expansions that, in principle, could be applied directly to the original integral. However, rather than do this, in each case the original function is replaced by a finite Chebyshev approximation, which
in turn allows the terms of each series to be computed using simple recurrence
relations. Of course, although the basic philosophy is similar, the actual techniques
used in each method are quite different, with the integration rule of Chapter
4 based on asymptotic expansions, whilst Smith’s rule is based on generalised
function theory and Hadamard finite part integrals.

A.2 An alternative technique for evaluating singular inte-
grals

An alternative technique for evaluating the integrals $N_n$ can be derived using some
simple results on indefinite integrals. Let

$$h(x) = (1 - x)^\alpha (1 + x)^\beta,$$  \hspace{1cm} (A.2.1)

then

$$(1 - x^2)h'(x) = [(\beta - \alpha) - (\beta + \alpha)x]h(x).$$  \hspace{1cm} (A.2.2)

Also let $p_n(x)$ be a polynomial of exact degree $n$ and, without loss of generality,
suppose that $-1 < \alpha, \beta < 0$. Then

$$\int h(x)p_n(x) \, dx = g_{n-1}(x)(1 - x^2)h(x) + K \int h(x) \, dx,$$  \hspace{1cm} (A.2.3)

where $g_{n-1}(x)$ is a polynomial of degree $n - 1$ and $K$ is a constant. Evaluating
this identity with the limits $-1$ and $1$ it follows that

$$\int_{-1}^{1} h(x)p_n(x) \, dx = K \int_{-1}^{1} h(x) \, dx = K \frac{2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}.$$  \hspace{1cm} (A.2.4)

Hence, to evaluate the integral $N_n$ it is only necessary to determine the constant
$K$. To do this differentiate (A.2.3) to give

$$h(x)p_n(x) = g_{n-1}(x)(1 - x^2)h(x)$$

$$+ g_{n-1}(x)(1 - x^2)h'(x) - g_{n-1}(x)2xh(x) + Kh(x).$$  \hspace{1cm} (A.2.5)
Using the relation (A.2.2) and setting \( p_n(x) = T_n(x) \) and \( g_{n-1}(x) = \sum_{j=0}^{n-1} c_j T_j(x) \) gives
\[
T_n(x) = (1 - x^2) \sum_{j=0}^{n-1} c_j T_j'(x) - (\beta - \alpha) \sum_{j=0}^{n-1} c_j T_j(x) - (\beta + \alpha + 2)x \sum_{j=0}^{n-1} c_j T_j(x) + K. \tag{A.2.6}
\]

Applying equations (4.3.18) and (4.3.22) leads to
\[
T_n(x) = \frac{1}{2} \sum_{j=1}^{n-1} c_j [T_{j-1}(x) - T_{j+1}(x)] - (\beta - \alpha) \sum_{j=0}^{n-1} c_j T_j(x)
- \frac{1}{2} (\beta + \alpha + 2) \sum_{j=0}^{n-1} c_j [T_{j+1}(x) + T_{j-1}(x)] + K. \tag{A.2.7}
\]

Equating coefficients of \( T_j(x) \) on both sides, the following recurrence relations are obtained
\[
c_{n-1} = -2/((\beta + \alpha + n + 1) \tag{A.2.8}
\]
\[
c_{n-2} = -2(\beta - \alpha)c_{n-1} / (\beta + \alpha + n) \tag{A.2.9}
\]
\[
c_{j-1} = [-2(\beta - \alpha)c_j + (j - \beta - \alpha - 1)c_{j+1}]/(\beta + \alpha + j + 1) \tag{A.2.10}
\]
\[
j = n - 2, \ldots, 1
\]
\[
K = - (\beta - \alpha)c_0 + (\beta + \alpha + 1)c_1 / 2. \tag{A.2.11}
\]

Hence the constant \( K \) can be determined recursively from the coefficients in the Chebyshev expansion of \( g_{n-1}(x) \).
Bibliography


