

Numerical Quadrature of Oscillatory and Non-Oscillatory Integrals

by

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A thesis submitted to the Faculty of Science and Agriculture, University of Fort Hare,

Alice

in fulfillment of the requirements for the degree of

MASTER OF SCIENCE

in

Applied Mathematics

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DEDICATION

I would like to dedicate this thesis to my fiancée Feziwe Peter and to my son Isphile for the support they offered me from the beginning to the completion of this thesis. I would also like to dedicate it to the memory of my beloved mother Thandeka who passed-on four months into my first year at the university, whose undying wish was always to see me and my siblings graduate. Finally, I would like to thank my supervisor Prof. G.E. Okecha for his guidance.

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ACKNOWLEDGEMENTS

I would like to extend my most profound gratitude to Prof. George E. Okecha for his guidance and undiminishing support throughout this research and writing of this dissertation. I would also like to express my thanks to Joel Struss for the tips on LaTeX for thesis writing. Last but not least, I thank all those who helped and supported me during this research, particularly my dearest father Mthuthuzeli.

ABSTRACT

In this dissertation we develop efficient new methods and techniques to numerically evaluate integrals of both oscillatory and non oscillatory kind. We have done a comprehensive literature review on the existing methods and made some modifications to them so as to cope with difficulties such as oscillations and strong singularities. In the numerical algorithms we have used mainly the MATLAB source code. Our results have been compared with well known methods by renowned authors in this field.

CHAPTER 1. Overview

Numerical integration is the problem of obtaining approximate values for a given, definite integral of the form:

$$\int_a^b f(x)dx \tag{1}$$

where $[a, b]$ may be finite, semi-infinite or infinite. It is well-known that there is abundance of general and sophisticated methods for obtaining values of integrals, and the question is, ‘Why then do we have to use numerical approximations to the definite integrals?’

As we read we shall find the answer to this question in the next Section.

1.1 Introduction

Integration has got various applications in the fields of physics, applied mathematics, tomography, engineering etc, hence the need for further research into the field of numerical integration. Various methods have been developed over the past eight decades and the most prominent are the Newton-Cotes and Gaussian methods.

To answer the question about the need for numerical integration, we recall the Fundamental Theorem of integral calculus to explain the fact that, mathematically sophisticated methods do not always work i.e. some integrals are quite difficult or almost

impossible to obtain their solutions in a closed form.

Consider the integral,

$$\int_a^b f(x)dx = F(b) - F(a) \quad (2)$$

where $F(x)$ is the antiderivative of $f(x)$. If the antiderivative is readily available and adequately simple, equation(2) can provide the most expeditious computation. Despite this seemingly easy approach, another challenge may arise. This can be in the form of expressing the analytical solution by means of a transcendental function.

Another fundamental reason for developing rules for approximate integration is that, in some instances, we are confronted with the problem of integrating experimental data. In such cases, theoretical methods may prove totally inapplicable. The key features that make any numerical method stand out from others are accuracy and the lack of undue expenditure of labour i.e. one needs to achieve good results (acceptable error) with minimal effort.

In this thesis, we develop numerical integration techniques from known numerical integration methods in an attempt to address two problems that have been declared, by consensus, as posing the greatest challenge to existing numerical integration methods and these are:

- i) Highly oscillatory integrals
- ii) Cauchy principal value integrals
- iii) Hadamard finite part integrals

In the next Section we examine and give a summary of several papers from a sample of publications in this field.

1.2 Literature Review

Over the past eight decades, numerical integration has become a field of interest for many researchers, not only in applied mathematics but in other fields as well. The beginnings of this field date as far back as the sixteenth century. It is quite clear that numerical integration existed long before the invention of computers. It was until the early 1950s that numerical integration boomed most probably due to the invention of powerful computers.

This was a major invention as it levelled the field for more sophisticated experiments. We will give extracts and summary from publications and journals by various authors on numerical integration of highly oscillatory integrals, Cauchy principal value integrals, and Hadamard finite part integrals. We shall also give a brief definition of numerical integration.

Most literature defines numerical integration as the problem of finding approximate values for integrals of the form

$$\int_a^b f(t)dt \tag{3}$$

Since this problem is important in applications, various methods have been developed for that purpose, for example, the Trapezoidal and Simpson's rule, and far much more complicated formulas by Gauss. The latter will be discussed in detail in Chapter Three. The common feature of those and other methods is that we first choose points in $[a, b]$, called nodes, and then approximate the unknown value of the integral by a linear combination of the values of the function $f(t)$ at the nodes. The nodes and the coefficients of such a linear combination depend on the method but not on the integrand $f(t)$. Key to any numerical method, is the accuracy of the approximation and one may want the accuracy to increase as the number of nodes increases.

Another key feature central to numerical integration, is the requirement for the integrand to be continuous in the range of integration. For now we will limit our discussion to cases of continuous functions, however we will give ways around the solution of integrands that are not continuous in Chapter Four.

This discussion suggests the introduction of a Banach space $X = [a, b]$ of all continuous real-valued functions on $J = [a, b]$, with norm defined by

$$\|f\| = \max_{t \in J} |f(t)| \quad (4)$$

We define the definite integral in (3) by means of a linear functional $I(f)$ on X as follows

$$I(f) = \int_a^b f(t) dt \quad (5)$$

To obtain a formula for numerical integration, we may proceed as follows, for each n we choose $n + 1$ real numbers

$$t_0^{(n)}, t_1^{(n)}, \dots, t_n^{(n)} \quad (\text{called nodes}) \quad (6)$$

such that

$$a \leq t_0^{(n)} < \dots < t_n^{(n)} \leq b$$

Then we can choose $n + 1$ real constants

$$\alpha_0^{(n)}, \dots, \alpha_n^{(n)} \quad (\text{called coefficients}) \quad (7)$$

(4)

and define linear functionals g_n on X by setting

$$I_n = \sum_{k=0}^n \alpha_k^{(n)} f_n(t_k^{(n)}) \quad (n=1,2,\dots) \quad (8)$$

This defines a numerical process of integration, the value I_n being an approximation to $I(f)$ in equation (5) and $f(t)$ is the given integrand. Each I_n is bounded since

$$|f(t_k^{(n)})| \leq \|f\|$$

by definition of the norm.

Consequently,

$$I_n \leq \sum_{k=0}^n |\alpha_k^{(n)}| |f(t_k^{(n)})| \leq \left(\sum_{k=0}^n |\alpha_k^{(n)}| \right) \|f\| \quad (9)$$

If we choose an arbitrary function $f_0 \in X$ such that $|f_0| \leq 1$ on J , we obtain

$$\|I_n\| = \sum_{k=0}^n |\alpha_k^{(n)}| \quad (10)$$

This has led to the use of orthogonal polynomials which possess some of these properties and these will be discussed in Chapter Two.

For a given function $f \in X$, formula (8) yields an approximate value I_n to I in (5). Our interest is in the accuracy as n increases, so for this reason we introduce the concept of convergence.

1.2.1 Definition (Convergence)

The numerical process of integration defined by (8) is said to be convergent for $f \in X$ if for f ,

$$I_n \rightarrow I \quad \text{as} \quad n \rightarrow \infty \quad (11)$$

where I is defined by equation (5).

A more detailed study of numerical integration methods is given in Chapter Three. Let us give a brief discussion of some numerical methods from a sample of published work over the past eight decades.

We start with the notable achievement by Louis Napoleon George Filon (1928) on the quadrature of oscillatory functions. Filon was at the forefront of the academics who derived quadrature rules for approximating oscillatory integrals.

Consider the integral

$$I(f) = \int_a^b f(t)e^{i\omega t} dt \quad , \quad \omega \gg 1 \quad (12)$$

Filon proposed a quadrature rule by approximating the function $f(t)$ by parabolic arcs. In Filon's method, the interval $[a, b]$ is divided into $2N$ subintervals of equal length h , where

$$h = \frac{b - a}{2N}$$

Over each double subinterval, $f(t)$ is approximated by a parabola obtained by interpolation to $f(t)$ at the mesh points. For parabolic $f(t)$, the Fourier integrals can be

computed explicitly by integration by parts. This program leads to the following approximate rules of integration.

Let

$$C_{2n} = \frac{1}{2}f(a) \cos \omega a + f(a+2h) \cos \omega(a+2h) + f(a+4h) \cos \omega(a+4h) + \cdots + \frac{1}{2}f(b) \cos \omega b \quad (13)$$

$$C_{2n-1} = f(a+h) \cos \omega(a+h) + f(a+3h) \cos \omega(a+3h) + f(a+5h) \cos \omega(a+5h) + \cdots + f(b-h) \cos \omega(b-h) \quad (14)$$

Similarly, define S_{2n} and S_{2n-1} as the corresponding sums formed from $f(t) \sin \omega t$. Further, let

$$\theta = \omega h = \frac{\omega(b-a)}{2N} \quad (15)$$

and

$$\alpha = \alpha(\theta) = \frac{(\theta^2 + \theta \sin \theta \cos \theta - 2 \sin^2 \theta)}{\theta^3} \quad (16)$$

$$\beta = \beta(\theta) = 2 \frac{[\theta(1 + \cos^2 \theta) - 2 \sin \theta \cos \theta]}{\theta^3} \quad (17)$$

$$\gamma = \gamma(\theta) = 4 \frac{(\sin \theta - \theta \cos \theta)}{\theta^3} \quad (18)$$

Then,

$$\int_a^b f(t) \cos \omega t dt \approx h \{ \alpha [f(b) \sin \omega b - f(a) \sin \omega a] + \beta C_{2n} + \gamma C_{2n-1} \} \quad (19)$$

$$\int_a^b f(t) \sin \omega t dt \approx h \{ -\alpha [f(b) \cos \omega b - f(a) \cos \omega a] + \beta S_{2n} + \gamma S_{2n-1} \} \quad (20)$$

Note that the expressions in equations (16), (17), and (18) are indeterminate when $\theta = 0$ and their use ought to be avoided in such a case. One may thus use the following Taylor expansions instead,

$$\alpha(\theta) = \frac{2}{45}\theta^2 - \frac{2}{315}\theta^5 + \frac{2}{4725}\theta^7 + \dots \quad (21)$$

$$\beta(\theta) = \frac{2}{3} + \frac{2}{15}\theta^2 + \frac{2}{105}\theta^4 + \frac{2}{567}\theta^6 + \dots \quad (22)$$

$$\gamma(\theta) = \frac{4}{3} - \frac{2}{15}\theta^2 + \frac{1}{210}\theta^4 - \frac{1}{11340}\theta^6 + \dots \quad (23)$$

For high oscillation it is advisable to keep the parameter θ smaller than 1.

Let E_s and E_c designate the respective errors in Filon's method for sine and cosine formulas.

If we set,

$$H(\theta) = \left| \frac{\sin \theta}{3\theta^2} + \frac{\cos \theta}{\theta^3} - \frac{\sin \theta}{\theta^4} \right| \quad (24)$$

$$M = \max_{a \leq t \leq b} |f^{(3)}(t)| \quad (25)$$

Then, assuming that $\theta < 1$, it has been shown[8] that

$$|E_s|, |E_c| \leq (b - a)MH(\theta)h^3 + O(h^4) \quad (26)$$

Filon's method was later on generalised by Luke[20] and Flinn[7]. Recently, Iserles and Norsett[13] presented a qualitative understanding of the extended Filon's method univariate setting.

Several authors have also shown interest in this topic, see for instance Håvie[[10],[11]], Hamming[9], Kruglikova[15], Evans and Chung[6].

Another method which has been celebrated in this field is the method due to David Levin[18]. This method numerically integrates the integral without any need to evaluate the moments, but uses a collocation technique.

Suppose we want to evaluate the integral,

$$I = \int_a^b f(t)e^{i\omega g(t)} dt \quad (27)$$

we take an arbitrary function F such that

$$\frac{d}{dx} [F(t)e^{i\omega g(t)}] = [F'(t) + i\omega g'(t)F(t)] e^{i\omega g(t)} = f(t)e^{i\omega g(t)} \quad (28)$$

Levin suggested that $F(t)$ be expressed by a linear combination of the bases functions $\{\phi_i(t)\}_{i=0}^n$ and collocate using $f(t)$ at the nodes $t_i \in [a, b]$, $i=0,1,2,\dots,n$.

Thus,

$$F(t) = \sum_{i=0}^n \alpha_i \phi_i(t) \quad (29)$$

Then,

$$F'(t_i) + i\omega g'(t_i)F(t_i) = f(t_i) \quad i=0,1,2,\dots,n \quad (30)$$

We then define,

$$I \approx \tilde{I} = F(b)e^{i\omega g(b)} - F(a)e^{i\omega g(a)} \quad (31)$$

Some authors have modified this method, see for instance Olver[26].

We now explore the methods for the evaluation of integrals with singularities. Bareiss and Neuman[2] suggested the following method of symmetric pairing.

Consider the integral,

$$I = \int_a^b f(t)dt \quad (32)$$

Assume that $f(t)$ is unbounded in the neighbourhood of $t = \lambda$ and the Cauchy principal value

$$\lim_{\epsilon \rightarrow 0^+} \left[\int_a^{\lambda-\epsilon} f(t)dt + \int_{\lambda+\epsilon}^b f(t)dt \right] \text{ exists} \quad (33)$$

Suppose $\lambda = 0$ and the integral is of the form $\int_{-a}^a f(t)dt$.

Suppose we set

$$g(t) = \frac{1}{2} [f(t) - f(-t)] \quad \text{and} \quad h(t) = \frac{1}{2} [f(t) + f(-t)], \quad (34)$$

then,

$$f(t) = g(t) + h(t) \quad (35)$$

where,

$g(t)$ is an odd function $g(t) = -g(-t)$ and $h(t)$ is an even function $h(t) = h(-t)$.

Hence we express,

$$\begin{aligned} \int_{-a}^{-\epsilon} f(t)dt + \int_{\epsilon}^a f(t)dt &= \int_{-a}^{-\epsilon} g(t)dt + \int_{\epsilon}^a g(t)dt + \int_{-a}^{-\epsilon} h(t)dt + \int_{\epsilon}^a h(t)dt \\ &= 2 \int_{\epsilon}^a h(t)dt \end{aligned} \quad (36)$$

Therefore,

$$\begin{aligned}
\int_{-a}^a f(t) dt &= 2 \lim_{\epsilon \rightarrow 0^+} \int_{\epsilon}^a h(t) dt \\
&= 2 \int_0^a h(t) dt \\
&= \int_0^a [f(t) + f(-t)] dt
\end{aligned} \tag{37}$$

The same strategy can be extended to Cauchy principal values over infinite interval.

We now briefly discuss the method of subtracting the singularity. Suppose we want to evaluate the integral of the form

$$I(f) = \int_a^b \frac{f(t)}{t - \lambda} dt \quad \lambda \in (a, b) \tag{38}$$

We may write,

$$\begin{aligned}
I(f) &= \int_a^b f(t) dt \\
&= \int_a^b \frac{f(t) - f(\lambda)}{t - \lambda} dt + f(\lambda) \int_a^b \frac{dt}{t - \lambda} \\
&= \int_a^b \frac{f(t) - f(\lambda)}{t - \lambda} dt + f(\lambda) \ln \frac{b - \lambda}{\lambda - a}
\end{aligned} \tag{39}$$

If we assume that the function

$$\phi(t, \lambda) = \frac{f(t) - f(\lambda)}{t - \lambda} \quad (40)$$

is of class $C^1[a, b]$ for fixed λ and variable t , then $\phi(\lambda, \lambda) = f'(\lambda)$ and the integral $\int_a^b \phi(t, \lambda) dt$ has no difficulties associated with it. For a more detailed description of these methods, the reader is referred to Monegato[22], Davis and Rabinowitz[4], Longman[19] and Stewart[31].

Our thesis is organised as follows. In Chapter Two we present theoretical background underlying numerical integration methods wherein we discuss the orthogonal polynomials and interpolation. In Chapter Three we discuss the numerical integration of Cauchy principal value integrals and Hadamard finite part integrals using Gauss-type methods. In Chapter Four we give the modified methods and techniques for evaluating Oscillatory integrals using Newton-Cotes quadrature. In Chapter Five we discuss numerical evaluation of Fourier type integrals using the collocation method. In Chapter Six we give our conclusion and pointers for future work.

CHAPTER 2. General Quadrature Theory

2.1 Interpolation

2.1.1 Introduction

Consider a family of functions of a single variable t , $\phi(t, a_0, \dots, a_n)$, having $n + 1$ parameters a_0, a_1, \dots, a_n whose values characterise the individual functions in this family. The interpolation of ϕ consists of determining the parameters a_i so that for $n + 1$ given real or complex pairs of numbers (t_i, f_i) , $i=0,1,\dots,n$ with $t_i \neq t_k$ for, $i \neq k$

$$\phi(t_i, a_0, a_1, \dots, a_n) = f_i, \quad i=0,1,\dots,n, \quad \text{holds} \quad (41)$$

We will call the pairs (t_i, f_i) support points, and the locations t_i support abscissas, and the values f_i support ordinates. At times, the values of derivatives of ϕ are also prescribed, in the case of Hermite interpolation.

This process is called a linear interpolation problem if ϕ depends linearly on the parameters a_i such that

$$\phi(t, a_0, \dots, a_n) \equiv a_0\phi_0(t) + a_1\phi_1(t) + \dots + a_n\phi_n(t) \quad (42)$$

This class of problems includes the classical polynomial interpolation given by:

$$\phi(t, a_0, \dots, a_n) \equiv a_0 + a_1t + \dots + a_nt^n \quad (43)$$

and the trigonometric interpolation given by:

$$\phi(t, a_0, \dots, a_n) \equiv a_0 + a_1e^{it} + \dots + a_ne^{int}, \quad i^2 = -1 \quad (44)$$

Polynomial interpolation is very important and it is the basis of several types of numerical integration formulae hence it forms the integral part of our thesis.

Trigonometric interpolation is used extensively for the numerical Fourier analysis of Time Series and cyclic phenomena in general. The class of linear interpolation problems also contains spline interpolation. Spline interpolation is a relatively new development of growing interest. It provides a valuable tool for representing empirical curves and for approximating complicated mathematical functions.

Two non linear interpolation schemes of importance are

Rational interpolation:

$$\phi(t, a_0, \dots, a_n, b_0, \dots, b_m) \equiv \frac{a_0 + a_1t + \dots + a_nt^n}{b_0 + b_1t + \dots + b_mt^m}, \quad m > n \quad (45)$$

Exponential interpolation:

$$\phi(t, a_0, \dots, a_n, \lambda_0, \dots, \lambda_n) \equiv a_0e^{\lambda_0t} + a_1e^{\lambda_1t} + \dots + a_ne^{\lambda_nt} \quad (46)$$

and this is used in radio active decay analysis. For a comprehensive discussion of these and related topics see Davis[4].

2.1.2 Interpolation by polynomials

Let Π_n be the set of all real or complex polynomials of degree not exceeding n . So

$$\text{Let } P(t) \in \Pi_n, \text{ i.e. } P(t) = a_0 + a_1t + \cdots + a_nt^n \quad (47)$$

Theorem 2.1.2.1 For $n + 1$ arbitrary support points (t_i, f_i) , $i=0,1,\dots,n$, $t_i \neq t_k$ for $i \neq k$, there exists a unique polynomial $P \in \Pi_n$ with $P(t_i) = f_i$, $i=0,1,\dots,n$.

Proof

Uniqueness:

For any two polynomials $P_1, P_2 \in \Pi_n$ with $P_1(t_i) = P_2(t_i) = f_i$, $i = 0, 1, \dots, n$, the polynomial $P = P_1 - P_2 \in \Pi_n$ has degree at most n , but it has at least $n + 1$ different zeros, namely t_i , $i = 0, 1, \dots, n$. P must therefore vanish identically, and thus $P_1 = P_2$.

Existence:

We will construct the interpolating polynomial P explicitly with the help of polynomials $L_i \in \Pi_n$, $i = 0, 1, \dots, n$ for which

$$L_i(t_k) = \delta_{ik} = \begin{cases} 1 & \text{if } i = k \\ 0 & \text{if } i \neq k \end{cases} \quad (48)$$

The following Lagrange polynomials satisfy the above conditions:

$$\begin{aligned} L_i(t) &= \frac{(t - t_0) \cdots (t - t_{i-1})(t - t_{i+1}) \cdots (t - t_n)}{(t_i - t_0) \cdots (t_i - t_{i-1})(t_i - t_{i+1}) \cdots (t_i - t_n)} \\ &= \frac{\omega(t)}{\omega'(t_i)(t - t_i)} \end{aligned}$$

with

$$\omega(t) = \prod_{i=0}^n (t - t_i) \tag{49}$$

The solution P of the interpolation problem can now be expressed directly in terms of the polynomials L_i , leading to the Lagrange interpolating formula:

$$\begin{aligned} P_n(t) &= \sum_{i=0}^n f(t_i)L_i(t) \\ &= \sum_{i=0}^n f(t_i) \prod_{\substack{k \neq i \\ k=0}}^n \frac{t - t_k}{t_i - t_k} \end{aligned} \tag{50}$$

It is sometimes useful to find several approximating polynomials say $P_1(t), P_2(t), \dots, P_n(t)$ and then choose the one that best suits the needs.

If the Lagrange polynomials are used, there is no constructive relationship between say $P_n(t)$ and $P_{n-1}(t)$, $n = 2, 3, \dots$. Each polynomial has to be constructed individually, and the work required to compute higher order polynomials involves many computations.

Hence we introduce Newton's divided differences to construct Newton interpolation polynomials that have a recursive pattern as follows:

$$\begin{aligned}
P_0(t) &= a_0 \\
P_1(t) &= a_0 + a_1(t - t_0) \\
P_2(t) &= a_0 + a_1(t - t_0) + a_2(t - t_0)(t - t_1) \\
&\vdots \\
P_N(t) &= a_0 + a_1(t - t_0) + \cdots + a_N \prod_{i=0}^{N-1} (t - t_i)
\end{aligned} \tag{51}$$

Consequently, the interpolating polynomial $P_N(t)$ is given by,

$$P_N(t) = a_0 + a_1(t - t_0) + \cdots + a_N \prod_{i=0}^{N-1} (t - t_i) \tag{52}$$

Theorem 2.1.2.2 If $f(t)$ is a polynomial of degree N , then

$$f[t_0, t_1, \dots, t_k] = 0 \quad \text{for } k > N$$

Proof

In view of the unique solvability of the interpolation problem (see Theorem 2.1.2.1), $P_N(t) = f(t)$ for $k \leq N$. The coefficients of t^k in $P_k(t)$ must therefore vanish for $k > N$ since the Newton's interpolation polynomial is recursive in nature and linear dependent. This coefficient, however, is given by $f[t_0, t_1, \dots, t_k]$ according to equations(51) and this completes the proof.

If the function $f(t)$ is sufficiently smooth, then its divided differences can also be defined for arguments t_i that coincide. In such cases the divided differences are defined by their derivatives at those particular points for instance,

$$f[t_i, t_i] = f'(t_i) \tag{53}$$

and in general $f[t_i, t_i, \dots, (n + 1)\text{times}] = \frac{1}{n!} f^{(n)}(t_i)$ on the assumption that $f \in C^n$.

2.1.3 The Error of Interpolation by Polynomials

Consider a given function $f(t)$ and certain of its values $f_i = f(t_i)$, $i = 0, 1, \dots, N$ which are to be interpolated. Our aim is to determine how best the interpolating polynomial $P_N(t)$ with $P_N(t_i) = f_i$, $i = 0, 1, \dots, N$ approximates $f(t)$ for arguments different from the support arguments t_i .

Theorem 2.1.3.1 If the function $f(t)$ has an $(N + 1)$ st derivative, then for every argument \bar{t} there exists a number ξ in the smallest interval $J[t_0, t_1, \dots, t_N, \bar{t}]$ which contains \bar{t} and all support abscissas t_i , satisfying

$$f(\bar{t}) - P_N(\bar{t}) = \frac{\omega(\bar{t})}{(N + 1)!} f^{(N+1)}(\xi) \quad (54)$$

where

$$\omega(t) = (t - t_0)(t - t_1) \cdots (t - t_N)$$

Proof

Let $P_N(t)$ be the polynomial which interpolates the function $f(t)$ at t_i , $i = 0, 1, \dots, n$, and suppose that $\bar{t} \neq t_i$. If $\bar{t} = t_i$, equation (54) follows immediately from Theorem (2.1.2.1) and the definition of $\omega(t)$. Suppose that $\bar{t} = t_i$, $i = 0, 1, \dots, N$, then we can find a constant K such that the function

$$F(t) = f(t) - P_N(t) - K\omega(t) \quad \text{vanishes for } t = \bar{t} \quad (55)$$

.

Consequently, $F(t)$ has at least $(N + 2)$ zeros $(t_0, t_1, \dots, t_N, \bar{t}) \in J[t_0, t_1, \dots, t_N, \bar{t}]$

By Rolle's theorem, applied repeatedly, $F'(t)$ has at least $(N + 1)$ zeros in the above inter-

val, $F''(t)$ at least N zeros, and finally $F^{(N+1)}(t)$ at least one zero $\xi \in J[t_0, t_1, \dots, t_N, \bar{t}]$.
 Since

$$P_N^{(N+1)}(t) = 0$$

We have

$$F^{(N+1)}(\xi) = 0 \Rightarrow f^{(N+1)}(\xi) - K(N+1)! = 0$$

Thus,

$$K = \frac{f^{(N+1)}(\xi)}{(N+1)!} \quad \text{and this completes the proof}$$

We may proceed further to derive an error term from the Newton's divided difference scheme as follows,

Let

$P_N(t)$ be the interpolating polynomial defined by equation (52). If in addition to the $(N+1)$ support points (t_i, f_i) , $f_i = f(t_i)$, $i = 0, 1, \dots, N$. We introduce an $(N+2)$ nd support point (t_{N+1}, f_{N+1}) , $t_{N+1} = \bar{t}$, $f_{N+1} = f(\bar{t})$ where $\bar{t} \neq t_i$, $i = 0, 1, \dots, N$

Then by the Newton's formula, we have

$$f(\bar{t}) = P_N(\bar{t}) = P_N(\bar{t}) + f[t_0, t_1, \dots, t_N, \bar{t}]\omega(\bar{t})$$

or

$$f(\bar{t}) - P_N(\bar{t}) = f[t_0, t_1, \dots, t_N, \bar{t}] \omega(\bar{t})$$

In view of theorem (2.1.3.1) and $\omega(\bar{t}) \neq 0$, we must have

$$f[t_0, t_1, \dots, t_N, \bar{t}] = \frac{f^{(N+1)}(\xi)}{(N+1)!} \quad \text{for some } \xi \in J[t_0, t_1, \dots, t_N, \bar{t}]$$

By extension this result leads to

$$f[t_0, t_1, \dots, t_N] = \frac{f^{(N)}(\xi)}{N!} \quad \text{for some } \xi \in J[t_0, t_1, \dots, t_N]$$

which relates the derivatives and the divided differences.

Theorem 2.1.3.2 Let $P_N(t)$ be the unique interpolating polynomial as defined in equation (52), then the N^{th} divided difference is given by $a_N = f[t_0, t_1, \dots, t_N]$. Let t_0, t_1, \dots, t_N be $(N+1)$ support abscissas, and let C be a simple closed rectifiable curve in the z -plane enclosing t_0, t_1, \dots, t_N . If the function $f(t)$ is analytic inside and on C , then

$$f[t_0, t_1, \dots, t_N] = \frac{1}{2\pi i} \int_C \frac{f(z)}{(z-t_0)(z-t_1)\cdots(z-t_N)} dz \quad (55)$$

Proof

The representation in equation(55) can be derived from the Hermite error formula given by

$$f(z) - P_N(z) = \frac{1}{2\pi i} \int_C \frac{\omega(z)f(t)}{\omega(t)(t-z)} dt \quad (56)$$

where

$$\omega(z) = \prod_{j=0}^N (z - t_j)$$

Using the Cauchy integral representation for $f(z)$ in equation (56), we obtain

$$P_N(z) = \frac{1}{2\pi i} \int_C \left\{ \frac{\omega(z) - \omega(t)}{z - t} \right\} \frac{f(t)}{\omega(t)} dt \quad (57)$$

Notice that the right hand side of equation (56) vanishes at the points t_j in a Hermite sense, and that the integral in equation (56) is a polynomial of degree at most N in z , and these observations show that the right hand side of equation (57) is the interpolation polynomial $P_N(z)$ by uniqueness of interpolation polynomial.

Now since,

$$\frac{\omega(z) - \omega(t)}{z - t} = z^N + \dots \quad (58)$$

we see that the coefficient a_N of z^N in $P_N(z)$ is just the integral

$$a_N = \frac{1}{2\pi i} \int_C \frac{f(t)}{\omega(t)} dt$$

or

$$f[t_0, t_1, \dots, t_N] = \frac{1}{2\pi i} \int_C \frac{f(z)}{\omega(z)} dz$$

and this completes the proof.

2.1.4 Hermite interpolation

Consider the real numbers $\xi_i, f_i^{(k)}, k = 0, 1, \dots, n_i - 1, i = 0, 1, \dots, m$, with $\xi_0 < \xi_1 < \dots < \xi_m$

The Hermite interpolation problem for these data consists of determining a polynomial P whose degree does not exceed n , where

$$n + 1 = \sum_{i=0}^m n_i \quad (58)$$

and which satisfies the following interpolation conditions:

$$P^{(k)}(\xi_i) = f_i^{(k)}, \quad k = 0, 1, \dots, n_i - 1, \quad i = 0, 1, \dots, m \quad (59)$$

This problem differs from interpolation of (2.1.2) in that it prescribes at each support abscissa ξ_i not only the value but also the first $n_i - 1$ derivatives of the desired polynomial. It is clear that the interpolation problem of (2.1.2) is the special case $n_i = 1, i = 0, 1, \dots, m$.

Theorem(2.1.4.1) For arbitrary numbers $\xi_0, \xi_1, \dots, \xi_m, f_i^{(k)}, k = 0, 1, \dots, n_i - 1, i = 0, 1, \dots, m$, there exists precisely one polynomial

$$P \in \prod_n, \quad n + 1 = \sum_{i=0}^m n_i \quad (60)$$

which satisfies condition (59).

Proof

Uniqueness

Consider the polynomials $P_1(t), P_2(t) \in \prod_n$ for which condition (59) holds and let $P(t) = P_1(t) - P_2(t)$

Since

$$P^{(k)}(\xi_i) = 0, \quad k = 0, 1, \dots, n_i - 1, \quad i = 0, 1, \dots, m \quad (61)$$

ξ_i is at least an n_i - *fold* root of $P(t)$, so that $P(t)$ has altogether $\sum n_i = n + 1$ roots, each counted according to its multiplicity.

Thus $P(t)$ must vanish identically since its degree is less than $n + 1$.

Existence

For equation (59) is a system of n linear equations for n unknown coefficients a_i of $P(t) = a_0 + a_1t + \dots + a_nt^n$. The matrix of this system is non-singular, because of the uniqueness of its solutions. Hence the linear system (59) has a unique solution for arbitrary right hand sides $f_i^{(k)}$.

Hermite interpolation polynomials can be given explicitly in a form analogous to the interpolation formula in equation (50) as follows:

The polynomial $P(t) \in \prod_n$ given by

$$P(t) = \sum_{i=0}^m \sum_{k=0}^{n_i-1} f_i^{(k)} L_{ik}(t) \quad (62)$$

satisfies equation (59). The polynomials $L_{ik}(t) \in \prod_n$ are generalised Lagrange polynomials see [3].

Theorem(2.1.4.2) Let the real function f be $n + 1$ times differentiable on the interval $[a, b]$, and consider $m + 1$ support abscissae $\xi_i \in [a, b]$, $\xi_0 < \xi_1 < \dots < \xi_m$. If the polynomial

$$P(t) \in \Pi_n, \quad \sum_{i=0}^m n_i = n + 1 \text{ exists}$$

and satisfies the interpolation condition (59), then to every $\bar{t} \in [a, b]$ there exists $\bar{\xi} \in J[\xi_0, \xi_1, \dots, \xi_m, \bar{t}]$

such that

$$f(\bar{t}) - P(\bar{t}) = \frac{\omega(\bar{t})}{(n + 1)!} f^{(n+1)}(\bar{\xi})$$

where

$$\omega(t) = (t - \xi_0)^{n_0} (t - \xi_1)^{n_1} \dots (t - \xi_m)^{n_m}$$

For a detailed theory on this Section the reader is referred to Burlish and Stoer[3].

2.2 Orthogonal Polynomials

Sets of orthogonal polynomials play a considerable role in the theory of numerical integration and for this reason it would be worthwhile to give some of their properties and relevant formulas.

Given a real linear space of continuous functions $X = C[a, b]$, for $f, g \in X$, define (f, g) as an inner product of f and g and let the following conditions be satisfied

a) $(f + g, h) = (f, h) + (g, h)$

b) $(\alpha f, g) = \alpha(f, g)$ for α scalar

c) $(f, g) = (g, f)$

d) $(f, f) > 0$ if $f \neq 0$

If f_0, f_1, \dots is a finite or infinite set of elements of X such that

$$(f_i, f_j) = 0, \quad i \neq j \quad (63)$$

then the set is called orthogonal.

A set of polynomials P_i of degree i which satisfies equation (63) is called a set of orthogonal polynomials with respect to the inner product (f, g) .

As part of our thesis work, we define the inner product as follows:

Let the weight function $\omega(t) \geq 0$ be Riemann-integrable over $[a, b]$ such that

$$\int_a^b \omega(t) dt \geq 0$$

Then, we define an inner product with respect to this weight function as

$$(f, g) = \int_a^b \omega(t) f(t) g(t) dt \quad (64)$$

The weight function must meet the following requirements.

1) $\omega(t) \geq 0$ is measurable on the finite or infinite interval $[a, b]$.

2) All moments $\mu_k = \int_a^b t^k \omega(t) dt$, $k = 0, 1, \dots$, exist and are finite.

3) For polynomials $h(t)$ which are non-negative on $[a, b]$, $\int_a^b \omega(t) h(t) dt = 0 \Rightarrow h(t) \equiv 0$.

We now state a theorem which establishes the existence of a sequence of mutually orthogonal polynomials, the system of orthogonal polynomials associated with the weight

function $\omega(t)$.

Let,

$$\bar{\prod}_n = \{p | p(t) = t^n + a_1 t^{n-1} + \cdots + a_n, n = 0, 1, 2, \dots\} \quad (65)$$

form the set of normed real polynomials of degree n , which is monic.

Theorem (2.2.1) There exist polynomials $p_n \in \bar{\prod}_n$, $n = 0, 1, 2, \dots$ such that

$$(p_i, p_n) = 0, \quad \text{for } i \neq n \quad (66)$$

These polynomials are uniquely defined by the recursions

$$p_{n+1}(t) = (t - \alpha_n)p_n(t) - \beta_n p_{n-1}(t), \quad n = 0, 1, 2, \dots \quad (67)$$

$$p_{-1}(t) = 0, \quad p_0(t) = 1 \quad (68)$$

where α_n and β_n are real positive constants, and

$$\alpha_n = \frac{(tp_n(t), p_n(t))}{(p_n(t), p_n(t))} \quad \text{for } n \geq 0 \quad (69)$$

$$\beta_n = \begin{cases} 0 & \text{for } n = 0 \\ \frac{(p_n(t), p_n(t))}{(p_{n-1}(t), p_{n-1}(t))} & \text{for } n \geq 1 \end{cases} \quad (70)$$

Proof

These polynomials can be constructed by a recursive technique known as the Gram-Schmidt orthogonalization process.

Let

$$\begin{aligned} h(t) &= p_{n+1}(t) - tp_n(t) \in \prod_n \\ &= (t^{n+1} + \dots) - t(t^n + \dots) \end{aligned} \tag{71}$$

Hence, $h(t)$ can be expanded in terms of the orthogonal set $\{p_i(t)\}_{i=0}^n$ as

$$\begin{aligned} h(t) &= \sum_{k=0}^n \frac{(h, p_k)}{(p_k, p_k)} p_k \\ &= \sum_{k=0}^n \frac{(p_{n+1} - tp_n, p_k)}{(p_k, p_k)} p_k \\ &= - \sum_{k=0}^n \frac{(tp_n, p_k)}{(p_k, p_k)} p_k \\ &= - \sum_{k=0}^n \frac{(p_n, tp_k)}{(p_k, p_k)} p_k \\ &= - \sum_{k=n-1}^n \frac{(p_n, tp_k)}{(p_k, p_k)} p_k \end{aligned} \tag{72}$$

In view of equations (69) and (70), and upon solving for $p_{n+1}(t)$, we obtain

$$p_{n+1}(t) = (t - \alpha_n)p_n(t) - \beta_n p_{n-1}(t) \quad (73)$$

and this completes the proof.

Corollary(2.2.2): $(p, p_n) = 0$ for all $p \in \prod_{n-1}$

Proposition(2.1.2.7): The roots $t_i, i = 1, 2, \dots, n$ of the n^{th} order orthogonal polynomial $p_n(t)$ are the eigenvalues of the Jacobi tridiagonal matrix J_n ,

$$J_n = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & 0 & 0 & \cdots & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & 0 & \cdots & 0 \\ 0 & \sqrt{\beta_2} & \ddots & \ddots & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & \vdots & \ddots & \ddots & \alpha_{n-1} & \sqrt{\beta_n} \\ 0 & \cdots & \cdots & \sqrt{\beta_n} & \alpha_n & \end{bmatrix} \quad (74)$$

Theorem(2.2.3)

The roots $t_i, i = 1, 2, \dots, n$ of $p_n(t)$ are real and simple. They all lie in the interval (a, b) .

Proof

Let t_1, t_2, \dots, t_m be the places where $p_n(t)$ changes signs in (a, b) . The polynomial

$$q(t) = \prod_{i=1}^m (t - t_i) \in \prod_m \quad (75)$$

is such that the product polynomial

$$q(t)p_n(t) = (t - t_1)(t - t_2) \cdots (t - t_m)p_n(t) \quad (76)$$

never changes signs in (a, b) .

Suppose that $m < n$, then by the orthogonality property with respect to the weight function $\omega(t)$ we have,

$$(p_n, q) = \int_a^b \omega(t)q(t)p_n(t)dt = 0 \quad (77)$$

The only possibility is that $n = m$ since $p_n(t)$ has at most n real zeros. Since $p_n(t)$ changes signs n times, we conclude that the roots of $p_n(t)$ are distinct.

Theorem 2.2.4 The $n \times n$ matrix

$$A = \begin{bmatrix} p_0(t_1) & \cdots & p_0(t_n) \\ \vdots & \cdots & \vdots \\ p_{n-1}(t_1) & \cdots & p_{n-1}(t_n) \end{bmatrix} \quad (78)$$

is non-singular for mutually distinct arguments t_i , $i = 1, 2, \dots, n$.

The classical orthogonal polynomials which we work with in the development of quadrature formulae are the Legendre and Chebyshev polynomials.

2.2.1 The Legendre Polynomials

Conventional symbol for the Legendre polynomials of the first kind: $P_n(t)$ where n is the order, interval: $[-1, 1]$

Weight: 1

Standardisation: $P_n(1) = 1$

Norm: $\int_{-1}^1 p_n(t)^2 dt = \frac{2}{2n+1}$

Inequality: $|P_n(t)| \leq 1$ for $t \in [-1, 1]$

Rodrigue's formula: $\frac{(-1)^n}{2^n n!} \frac{d^n}{dt^n} (1-t^2)^n = P_n(t)$

Recurrence relation: $(n+1)P_{n+1}(t) = (2n+1)tP_n(t) - nP_{n-1}(t)$

Conventional symbol for the Legendre polynomial of the second kind: $Q_n(t)$

$\int_{-1}^1 \frac{P_n(t)}{t-z} dt = -2Q_n(z)$.

$Q_n(t)$ satisfies same differential equation as $P_n(t)$.

2.2.1.1 Finding the zeros of the Legendre polynomial $P_n(t)$

Consider the recurrence relation

$$p_{n+1}(t) = (t - \alpha_n)p_n(t) - \beta_n p_{n-1}(t) \quad (79)$$

We recall that the recurrence relation for the Legendre polynomials is given by

$$(n+1)P_{n+1}(t) = (2n+1)tP_n(t) - nP_{n-1}(t) \quad (80)$$

The leading coefficient for the Legendre polynomials is $\frac{(2n)!}{2^n (n!)^2}$.

Now let $p_n(t) = \frac{2^n (n!)^2}{(2n)!} P_n(t)$ and substitute in equation (80), we obtain

$$\frac{(n+1)(2(n+1))!}{((n+1)!)^2 2^{n+1}} p_{n+1}(t) = \frac{(2n+1)(2n)!}{(n!)^2 2^n} p_n(t) - \frac{n(2(n-1))!}{((n-1)!)^2 2^{n-1}} p_{n-1}(t) \quad (81)$$

Making $p_{n+1}(t)$ the subject of the formula, we obtain

$$p_{n+1}(t) = \frac{(2n+1)(2n)!((n+1)!)^2 2^{n+1}}{(n!)^2 2^n (n+1)(2(n+1))!} p_n(t) - \frac{n(2(n-1))!((n+1)!)^2 2^{n+1}}{((n-1)!)^2 2^{n-1} (n+1)(2(n+1))!} p_{n-1}(t) \quad (82)$$

Upon simplifying equation (82) we obtain

$$p_{n+1}(t) = t p_n(t) - \frac{n^2}{4n^2 - 1} p_{n-1}(t) \quad (83)$$

Comparing equation (79) with (83), we conclude that

$$\alpha_n = 0 \quad \text{and} \quad \beta_n = \frac{n^2}{4n^2 - 1} \quad (84)$$

We then use these recurrence coefficients in the tridiagonal matrix J_n and the MATLAB code is in Appendix A.

The Chebyshev Polynomials: The conventional symbol for the Chebyshev polynomials of the first kind is $T_n(t)$, where n is the degree of the polynomial.

By definition $T_n(t) = \cos(n \cos^{-1}(t))$

Recurrence relation: $T_{n+1}(t) = 2tT_n(t) - T_{n-1}(t)$, $T_0 = 1$, $T_1 = t$

Interval: $[-1,1]$

Weight: $\frac{1}{\sqrt{1-t^2}}$

Standardisation: $T_n(1) = 1$

$T_n(t)$ is a solution of the differential equation,

$$(1-t^2)y'' - ty' + n^2y = 0, \quad n = 0, 1, \dots, \quad y = T_n(t)$$

In the next section we present Gaussian quadrature.

CHAPTER 3. Gaussian Quadrature with Applications

3.1 Gaussian Quadrature

Gaussian quadrature scheme is based on the weights and abscissas that are determined by imposing the constraint that if $f(t)$ is a polynomial of specified order, the quadrature sum must be the exact value of the integral.

That is, for N -point Gaussian quadrature scheme,

$$\int_a^b \omega(t)f(t)dt = \sum_{i=1}^N w_i f(t_i) \quad (85)$$

must be exact if $f(t)$ is a polynomial of degree $\leq 2N - 1$. The weighting function $\omega(t)$ is a non-negative and measurable on the interval $[a, b]$. The particular form of quadrature scheme being used depends on the form of $\omega(t)$. The simplest form of a polynomial of order k is t^k . Thus the Gaussian quadrature scheme requires that

$$I(f) = \int_a^b \omega(t)t^k dt = \sum_{i=1}^N w_i t_i^k \approx I_k(f) \quad (86)$$

be exact for certain values of k . Since $2N$ parameters are to be determined, namely (Nw_i 's and Nt_i 's), so $2N$ equations are needed to solve for them. Thus k can range over the lowest $2N$ values, $0 \leq k \leq 2N - 1$. Therefore for N -point Gaussian quadrature scheme, the quadrature sum will be the exact value of the integral if $f(t)$ is a polynomial of order $2N - 1$ or lower. The $2N - 1$ equations expressed in equation (86) are non-

linear and complicated to solve. To make the solution easier we propose a method for determining the abscissas separately from the weights.

Theorem(3.1.2) Let $\omega(t)$ be a positive weight function and p_0, p_1, \dots, p_n a set of orthogonal polynomials with respect to the inner product $(p_i, p_j) = \int_a^b \omega(t)p_i(t)p_j(t)dt$ such that for each $k = 0, 1, \dots, n$, the order of $p_k(t)$ is equal to k . Let t_1, t_2, \dots, t_n be the zeros of $p_n(t)$, where $a < t_1 < t_2 < \dots < t_n < b$. There exist positive constants $\lambda_1, \lambda_2, \dots, \lambda_n$ such that,

$$\int_a^b \omega(t)f(t)dt = \sum_{k=1}^n \lambda_k f(t_k) \quad \text{whenever } f \in \prod_{2n-1} \quad (87)$$

.

Proof

Let $f \in \prod_{2n-1}$ and define $q(t) \in \prod_{n-1}$ by,

$$q(t) = \sum_{k=1}^n f(t_k)L_k(t) \quad (88)$$

where $L_k(t)$ is the Lagrange polynomial. Since the Lagrange polynomial satisfies

$$L_k(t_j) = \delta_{kj} = \begin{cases} 0 & \text{if } k \neq j \\ 1 & \text{if } k = j \end{cases} \quad (89)$$

we have $q(t_k) = f(t_k)$ for $k = 1, 2, \dots, n$. Clearly, $f(t) - q(t) \in \prod_{2n-1}$ and has zeros t_1, t_2, \dots, t_n . Since these are precisely the zeros of the n^{th} order orthogonal polynomial, we let

$$f(t) - q(t) = p_n(t)r_{n-1}(t), \quad r_{n-1}(t) \in \prod_{n-1} \quad (90)$$

So,

$$\begin{aligned}
\int_a^b f(t)\omega(t)dt &= \int_a^b \{q(t) + p_n(t)r_{n-1}(t)\}\omega(t)dt \\
&= \int_a^b q(t)\omega(t)dt \quad \text{by orthogonality} \\
&= \int_a^b \sum_{k=1}^n f(t_k)L_k(t)\omega(t)dt \quad \text{by equation (91)} \\
&= \sum_{k=1}^n f(t_k) \int_a^b L_k(t)\omega(t)dt
\end{aligned}$$

Upon letting $\int_a^b L_k(t)\omega(t)dt = \lambda_k$, we obtain the desired results and this completes the proof.

3.1.1 Finding the weights

Consider the polynomial

$$\mu_k(t) = \frac{p_n(t)}{(t - t_k)p'_n(t_k)} \quad (92)$$

where $p_n(t)$ is the n^{th} order orthogonal polynomial. Observe that $\mu_k(t_j) = \delta_{kj}$.

Since $\mu_k(t)$ is a polynomial of order $n - 1$, we can write $q(t)$ in the form

$$q(t) = \sum_{k=1}^n f(t_k)\mu_k(t) \quad (93)$$

In view of equations (90) and (93), we have

$$f(t) = p_n(t)r_{n-1}(t) + \sum_{k=1}^n f(t_k)\mu_k(t) \quad (94)$$

Since $f(t)$ is a polynomial of order $2n - 1$ and in view of Theorem (3.1.2), the following equation

$$\int_a^b f(t)\omega(t)dt = \sum_{k=1}^n w_k f(t_k) \quad (95)$$

is exact.

Upon substituting equation (94) into (95), we obtain

$$\int_a^b f(t)\omega(t)dt = \int_a^b p_n(t)r_{n-1}(t)\omega(t)dt + \sum_{k=1}^n f(t_k) \int_a^b \mu_k(t)\omega(t)dt \quad (96)$$

Thus, in view of equation (95) and the orthogonality property, we have

$$\sum_{k=1}^n w_k f(t_k) = \sum_{k=1}^n f(t_k) \int_a^b \mu_k(t)\omega(t)dt \quad (97)$$

Hence, we conclude that

$$w_k = \int_a^b \mu_k(t)\omega(t)dt \quad (98)$$

3.2 Gauss Legendre Quadrature

The Legendre polynomials satisfy the orthogonality property on the interval $[-1, 1]$ with the weighting function $\omega(t) = 1$. Without any loss of generality, we shall use this interval since any finite interval can be linearly transformed to this interval.

Therefore, the Gauss Legendre rule is given by

$$\int_{-1}^1 f(t)\omega(t)dt \approx \sum_{k=1}^n w_k f(t_k) \quad (99)$$

where the t'_k s are the roots of the n^{th} order Legendre polynomial or rather the eigenvalues of the Jacobi matrix J_n .

The weights are given by equation (98) with $\phi_n(t) = P_n(t)$ the n^{th} order Legendre polynomial of the first kind.

Thus,

$$\begin{aligned} w_k &= \int_{-1}^1 \frac{P_k(t)}{(t-t_k)P'_k(t_k)} dt \\ &= \frac{1}{P'_k(t_k)} \int_{-1}^1 \frac{P_k(t)}{(t-t_k)} dt \\ &= -2 \frac{Q_k(t_k)}{P'_k(t_k)} \end{aligned} \quad (100)$$

where $Q_k(t)$ is the k^{th} order Legendre polynomial of the second kind.

3.3 Evaluation of Cauchy Principal Value integrals

In this Section we present numerical quadrature of Cauchy Principal Value(CPV) integrals using a modified Gauss-Legendre rule. Various cases of CPV integrals are considered and the numerical examples have been presented.

Consider the CPV integrals of the form

$$I(f, \lambda) = \int_{-1}^1 \frac{f(x)}{(x-\lambda_1)^\alpha(x-\lambda_2)^\beta} dx, \quad \lambda_1, \lambda_2 \in (-1, 1), \lambda_1 \neq \lambda_2, \quad \alpha, \beta \geq 0 \quad (101)$$

We assume that $f(x) \in C^1[-1, 1]$ and $\lambda_i \in \Re$ for $i=1, 2, \dots$

3.3.1 Subtraction of singularity (case $\alpha = 1, \beta = 0$)

Suppose we want to compute

$$I(f, \lambda) = \int_{-1}^1 \frac{f(x)}{x - \lambda_1} dx, \quad \lambda_1 \in (-1, 1) \quad (102)$$

Following Davis and Rabinowitz[4,p148], we have

$$\begin{aligned} I(f, \lambda_1) &= \int_{-1}^1 \frac{f(x)}{x - \lambda_1} dx \\ &= \int_{-1}^1 \frac{f(x) - f(\lambda_1)}{x - \lambda_1} dx + \int_{-1}^1 \frac{f(\lambda_1)}{x - \lambda_1} dx \\ &= \int_{-1}^1 \frac{f(x) - f(\lambda_1)}{x - \lambda_1} dx + f(\lambda_1) \ln \left\{ \frac{1 - \lambda_1}{1 + \lambda_1} \right\} \end{aligned} \quad (103)$$

If we assume that $f(x)$ satisfies the *Holder* condition then,

$$\phi(x, \lambda_1) = \frac{f(x) - f(\lambda_1)}{x - \lambda_1} \in C^1[-1, 1] \quad (104)$$

and

$$\phi(\lambda_1, \lambda_1) = f'(\lambda_1)$$

Equation (103) becomes relatively easy to solve and one may use any quadrature rule which does not use λ_1 as a node. In our case we use the $(n + 1)$ point Gauss- Legendre rule.

Thus,

$$I_n(f, \lambda_1) = \sum_{j=0}^n w_j \phi(x_j, \lambda_1) + f(\lambda_1) \ln \frac{1 - \lambda_1}{1 + \lambda_1} \quad (105)$$

where $\{x_j\}_{j=0}^n$ are the roots of the $(n+1)^{th}$ order Legendre polynomial of the first kind $P_{n+1}(x)$.

3.3.2 Hadamard Finite Part Integral (case $\alpha = 2, \beta = 0$)

Consider,

$$I(f, \lambda_1) = \rlap{-}\int_{-1}^1 \frac{f(x)}{(x - \lambda_1)^2} dx, \quad \lambda_1 \in (-1, 1) \quad (106)$$

which is a strongly singular valued integral since $\alpha > 1$. Suppose that $f(x)$ is a real valued function defined on the interval $[-1, 1]$, then if the limit,

$$I(f, \lambda_1) = \lim_{\epsilon \rightarrow 0} \left\{ \int_{-1}^{\lambda_1 - \epsilon} \frac{f(x)}{(x - \lambda_1)^2} dx + \int_{\lambda_1 + \epsilon}^1 \frac{f(x)}{(x - \lambda_1)^2} dx - 2 \frac{f(x)}{\epsilon} \right\} \quad (107)$$

exists and is finite, we say that the integral $I(f, \lambda_1)$ exists in the Hadamard finite part sense.

If we express equation (106) in the form:

$$\begin{aligned} I(f, \lambda_1) &= \rlap{-}\int_{-1}^1 \frac{f(x) - f(\lambda_1)}{(x - \lambda_1)^2} dx + \rlap{-}\int_{-1}^1 \frac{f(\lambda_1)}{(x - \lambda_1)^2} dx \\ &= \rlap{-}\int_{-1}^1 \frac{f(x) - f(\lambda_1)}{(x - \lambda_1)} \frac{1}{x - \lambda_1} dx + \rlap{-}\int_{-1}^1 \frac{f(\lambda_1)}{(x - \lambda_1)^2} dx \end{aligned} \quad (108)$$

and if we set

$$g(x) = \frac{f(x) - f(\lambda_1)}{x - \lambda_1} \quad (109)$$

we obtain,

$$I(f, \lambda_1) = \int_{-1}^1 \frac{g(x)}{x - \lambda_1} dx + f(\lambda_1) \int_{-1}^1 \frac{dx}{(x - \lambda_1)^2} \quad (110)$$

Expressing $g(x)$ in a series of Legendre polynomials $P_k(x)$ we obtain,

$$g(x) = \sum_{k=0}^{\infty} A_k P_k(x) \quad (111)$$

where

$$A_k = \frac{2k+1}{2} \int_{-1}^1 g(x) P_k(x) dx \quad (112)$$

see Spiegel[30,p243].

One may evaluate A_k 's by using a collocation method as follows,

$$\sum_{k=0}^n A_k P_k(x_j) = g(x_j); \quad j = 0, 1, 2, \dots, n \quad (113)$$

where we have truncated the infinite series in equation (111) and assumed that $|A_{n+1}| \approx 0$. Then equation(113) may be written in matrix form as

$$PA = G$$

where

$$A = [A_0, A_1, \dots, A_{n-1}, A_n]^T$$

$$G = [g(x_0), g(x_1), \dots, g(x_{n-1}), g(x_n)]^T$$

and

$$P = \begin{bmatrix} P_0(x_0) & P_1(x_0) & \dots & P_n(x_0) \\ P_0(x_1) & P_1(x_1) & \dots & P_n(x_1) \\ \vdots & \vdots & \dots & \vdots \\ P_0(x_{n-1}) & P_1(x_{n-1}) & \dots & P_n(x_{n-1}) \\ P_0(x_n) & P_1(x_n) & \dots & P_n(x_n) \end{bmatrix}$$

Since matrix P is invertible by Theorem(2.2.4), we thus have

$$A = P^{-1}G \quad (114)$$

Nevertheless, provided $g \in C[-1, 1]$, A_k may be obtained through a standard quadrature rule, but may be a cumbersome exercise.

Substituting equation(111) into (110) we obtain,

$$\begin{aligned} I(f, \lambda_1) &= \int_{-1}^1 \frac{\sum_{k=0}^{\infty} A_k P_k(x)}{x - \lambda_1} dx + f(\lambda_1) \int_{-1}^1 \frac{dx}{(x - \lambda_1)^2} \\ &= \sum_{k=0}^{\infty} A_k \int_{-1}^1 \frac{P_k(x)}{x - \lambda_1} dx + 2 \frac{f(\lambda_1)}{\lambda_1^2 - 1} \\ &= -2 \lim_{n \rightarrow \infty} \sum_{k=0}^n A_k Q_k(\lambda_1) + 2 \frac{f(\lambda_1)}{\lambda_1^2 - 1} \end{aligned} \quad (115)$$

and this is our first quadrature rule.

From Abramowitz and Stegun[1]

$$\int_{-1}^1 \frac{P_n(x)}{x - \lambda} dx = -2Q_n(\lambda) \quad (116)$$

where $Q_n(x)$ is the n^{th} order Legendre function of the second kind.

Alternatively, one may substitute equations (111) and (112) into (110) and in view of equation (116) we obtain,

$$\begin{aligned} I(f, \lambda_1) &= \sum_{k=0}^{\infty} -2A_k Q_k(\lambda_1) + 2 \frac{f(\lambda_1)}{\lambda_1^2 - 1} \\ &= - \sum_{k=0}^{\infty} (2k + 1) Q_k(\lambda_1) \int_{-1}^1 g(x) P_k(x) dx + 2 \frac{f(\lambda_1)}{\lambda_1^2 - 1} \end{aligned}$$

For numerical simplicity, we truncate the series in equation (117) and apply the $(n + 1)$ point Gauss-Legendre rule to the integral to obtain,

$$I(f, \lambda_1) = - \sum_{j=0}^n \sum_{k=0}^N g(x_j) P_k(x_j) w_j (2k + 1) Q_k(\lambda_1) + 2 \frac{f(\lambda_1)}{\lambda_1^2 - 1} \quad (118)$$

which is now our second quadrature rule.

3.3.3 The integrand has two simple poles (case $\alpha=\beta=1$)

Consider the integral with a cluster of simple poles,

$$I(f, \lambda) = \int_{-1}^1 \frac{f(x)}{(x - \lambda_1)(x - \lambda_2)} dx \quad (119)$$

Several authors have investigated this kind of integral, for instance, see Hunter[12], McNamee[21], Okecha[24]. We will therefore give an exposition of these methods.

Let

$$g(x) = \frac{f(x)}{(x - \lambda_1)(x - \lambda_2)} \quad (120)$$

, and $g(z)$ be a function of complex variable z , which is analytic in some region γ containing the interval $[-1,1]$ except at a finite number of simple poles z_r , $r = 1, 2, \dots, p$

inside $[-1,1]$. We denote the residues at these poles by R_r .

Considering the findings due to McNamee[21] and applying a modified residue theorem to the Contour integral,

$$\frac{1}{2\pi i} \int_{\gamma} \frac{g(z)}{(z-x)P_n(x)} dz \quad (121)$$

we obtain,

$$g(x) = \sum_{j=1}^n \frac{P_n(x)g(x_j)}{(x-x_j)P'_n(x_j)} + \sum_{r=1}^p \frac{P_n(x)R_r}{(x-z_r)P_n(z_r)} + \frac{P_n(x)}{2\pi i} \int_{\gamma} \frac{g(z)}{(z-x)P_n(z)} dz \quad (122)$$

Integrating over $[-1,1]$ we have,

$$I(f, \lambda) = \sum_{j=1}^n w_j g(x_j) + \sum_{r=1}^p \frac{R_r}{P_n(z_r)} Q_{n,r} + E_n \quad (123)$$

where

$$w_j = \int_{-1}^1 \frac{P_n(x)}{(x-x_j)P'_n(x_j)} dx$$

$$Q_{n,r} = \int_{-1}^1 \frac{P_n(x)}{x-z_r} dx$$

$$E_n = \frac{1}{2\pi i} \int_{\gamma} \frac{g(z)}{P_n(z)} dz \int_{-1}^1 \frac{P_n(x)}{z-x} dx \quad (124)$$

Equation (123) is limited to a case whereby the nodes do not coincide with one of the poles, however, equation (123) may be modified to suit a case when one of the nodes coincides with one of the poles, see Hunter[12].

3.4 The New Approach to case 3.3.3

Let

$$p_\lambda(x) = (x - \lambda_1)(x - \lambda_2) \quad (125)$$

Then it can be shown by means of partial fractions that

$$\frac{1}{p_\lambda(x)} = \sum_{i=1}^2 \frac{1}{p'_\lambda(\lambda_i)(x - \lambda_i)} \quad (126)$$

Substitute equation (126) into (119), we obtain,

$$I(f, \lambda) = \sum_{i=1}^2 \frac{1}{p'_\lambda(\lambda_i)} \int_{-1}^1 \frac{f(x)}{x - \lambda_i} dx \quad (127)$$

Upon subtracting the singularity, we obtain

$$I(f, \lambda) = \sum_{i=1}^2 \frac{1}{p'_\lambda(\lambda_i)} \int_{-1}^1 \frac{f(x) - f(\lambda_i)}{x - \lambda_i} dx + \sum_{i=1}^2 \frac{f(\lambda_i)}{p'_\lambda(\lambda_i)} \int_{-1}^1 \frac{dx}{x - \lambda_i} \quad (128)$$

Letting,

$$f(x) - f(\lambda_i) = \sum_{k=0}^n A_k P_k(x)$$

We obtain

$$I(f, \lambda) = -2 \sum_{i=1}^2 \sum_{k=0}^n \frac{1}{p'_\lambda(\lambda_i)} A_k Q_k(\lambda_i) + \sum_{i=1}^2 \frac{f(\lambda_i)}{p'_\lambda(\lambda_i)} \ln \left(\frac{1 - \lambda_i}{1 + \lambda_i} \right) \quad (129)$$

3.5 Numerical experiments

For the MATLAB code see Appendix A:

Example 1

Consider the integral,

$$I = \int_0^1 \frac{e^{-x}}{x - 0.375} dx = e^{-0.375} \{Ei(0.375) + E_1(1 - 0.375)\}$$

where $E_i(x)$ is the exponential integral function and $E_1(x)$ is the Weber function.

This integral was considered by Kutt[16].

By using, the interval tranformation from $[0, 1]$ to $[-1, 1]$ we obtain:

$$I = e^{-0.5} \int_{-1}^1 \frac{e^{-0.5x}}{x + 0.25} dx$$

By applying equation (105) with $n = 5$ we obtain:

Kutt[16]	OurMethod
-0.3037427810772036	-0.303742781077618

Example 2

Consider the integral,

$$I = \int_{-1}^1 \frac{(25 - x^2)^{-\frac{1}{2}}}{(x - 0.5)^2} dx = -0.532215122267867$$

This integral was considered by Paget[26]

By applying equation (118) with $n = 5$ and $N = 5$, we obtain

$$I \approx I_n = -0.532215119319332$$

Example 3

We again consider the integral,

$$I = \int_{-1}^1 \frac{dx}{(x - \frac{1}{2})(x + \frac{1}{2})} = -2.197224577336220$$

Applying equation (129) with $n = 4$, we obtained

$$I = -2.197224577336220$$

CHAPTER 4. Newton-Cotes Quadrature with Applications

The integration formulas of Newton-Cotes are obtained by replacing the integrand with a suitable interpolating polynomial say $h(t)$ and then approximate as,

$$\int_a^b f(t)dt \approx \int_a^b h(t)dt \quad (130)$$

This quadrature is based on forming a uniform partition of the closed interval $[a, b]$ given by

$$t_i = a + ih, \quad i = 0, \dots, n \quad \text{with step size } h = \frac{(b-a)}{n}, n > 0 \text{ integer} \quad (131)$$

Let $h_n(t) = \prod_n$ be the interpolating polynomial such that

$$h_n(t_i) = f_i = f(t_i) \quad \text{for } i = 0, 1, \dots, n \quad (132)$$

By using Lagrange's interpolation formula (50) and introduction of a new variable x such that $t = a + hx$, we obtain

$$L_i(t) = \prod_{\substack{k=0 \\ k \neq i}}^n \frac{x-k}{i-k} = \psi_i(x) \quad (133)$$

Let,

$$h_n(t) = \sum_{i=0}^n f_i L_i(t)dt \quad (134)$$

Upon integrating equation (134), we obtain

$$\begin{aligned}
\int_a^b h_n(t)dt &= \sum_{i=0}^n f_i \int_a^b L_i(t)dt \\
&= h \sum_{i=0}^n f_i \int_{t_0}^{t_n} \psi_i(x)dx \\
&= h \sum_{i=0}^n f_i \alpha_i
\end{aligned} \tag{135}$$

where the weights $\alpha_i = \int_0^n \psi_i(x)dx$ depend on n only and not on the function f to be integrated nor on the end points of the integration range.

4.1 The Trapezoidal rule

If $n = 1$ in equation (135) we obtain the trapezoidal rule as follows

$$\begin{aligned}
\int_a^b h_1(t)dt &= h \sum_{i=0}^1 f_i \alpha_i \\
&= h \{f_0 \alpha_0 + f_1 \alpha_1\} \\
&= h \left\{ f(t_0) \int_0^1 \frac{x-1}{0-1} dx + f(t_1) \int_0^1 \frac{x-0}{1-0} dx \right\} \\
&= h \left\{ f(t_0) \frac{1}{2} + f(t_1) \frac{1}{2} \right\} \\
&= \frac{h}{2} \{f(t_0) + f(t_1)\}
\end{aligned} \tag{136}$$

in the interval $[t_0, t_1]$ of the partition $t_i = a + ih, i = 0, 1, \dots, n$ and $h = \frac{b-a}{n}$

The rule may be extended to a composite rule, which involves partitioning the entire interval $[a, b]$ into a finite number of subintervals $[t_i, t_{i+1}]$ with $t_i = a + ih, i =$

$0, 1, \dots, n$ and $h = \frac{b-a}{n}$

For the entire interval $[a, b]$, we obtain the following approximate rule

$$T(f) = h \frac{f(a) + f(b)}{2} + h \sum_{i=1}^{n-1} f(a + ih) \quad (137)$$

If we let $n = 2$ we obtain The Simpson's rule as follows,

$$\alpha_0 = \int_0^2 \frac{(t-1)(t-2)}{(0-1)(0-2)} dt = \frac{1}{2} \int_0^2 (t^2 - 3t + 2) dt = \frac{1}{3}$$

$$\alpha_1 = \int_0^2 \frac{(t-0)(t-2)}{(1-0)(1-2)} dt = - \int_0^2 (t^2 - 2t) dt = \frac{4}{3}$$

$$\alpha_2 = \int_0^2 \frac{(t-0)(t-1)}{(2-0)(2-1)} dt = \frac{1}{2} \int_0^2 (t^2 - t) dt = \frac{1}{3}$$

Thus, $S(f) = \frac{h}{3} [f_0 + 4f_1 + f_2]$

4.2 Evaluation of Oscillatory integrals by integrating between the zeros

4.2.1 Newton-Cotes formula

In this Section we evaluate oscillatory integrals using composite trapezoidal rule based on the zeros of the oscillatory kernel of the integrand. We also apply Euler's transformation method. Some relevant numerical examples have been presented together with their respective numerical results to validate our method.

Our aim is to find a suitable approximation to the integrals of the form:

$$I(f, k) = \int_0^\infty f(x)k(x)dx, \quad 0 \leq x < \infty \quad (138)$$

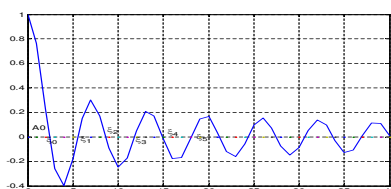
where $k(x)$ is an oscillatory weight function and $f(x)$ is well behaved and exponentially decaying in the interval $[0, \infty)$.

Here we determine the zeros of the integrand and then integrate between the successive zeros of the integrand. It has to be noted that by partitioning the integral, we successfully circumvent the possibility of having an oscillation between any two successive zeros. This reduces the problem into that of computing a series of well behaved partial integrals.

Let $0 < \xi_0 < \xi_1 < \dots < \xi_n < \dots < \infty$ be a partition D of $[0, \infty)$. Without any loss of generality, we assume in the rest of this paper, ξ_i for $i = 0, 1, 2, \dots$, to be the zeros of the integrand in question, without ruling out the possibility of 0 being a zero of the integrand.

We partition the integral as follows

Figure 4.1 zeros of an oscillatory function $k(x)$



$$I(f, k) = \int_0^{\xi} f(x)k(x)dx + \int_{\xi}^{\infty} f(x)k(x)dx, \xi = \max_{|\xi_i|}, i = 0, 1, 2, \dots \quad (139)$$

where ξ is the largest zero of the integrand which is adequate to permit truncation. The solution of the first integral of equation (139) is found by integrating between the successive zeros of the integrand, and the second part of the integral is taken to be negligible as $\xi \rightarrow \infty$.

Thus we have assumed that

$$\lim_{\xi \rightarrow \infty} \int_{\xi}^{\infty} f(x)k(x)dx \longrightarrow 0 \quad (140)$$

Consider the first part of the integral in equation (139)

$$\begin{aligned} I(f, k) &\approx \int_0^{\xi} f(x)k(x)dx \\ &= \int_{D_1} f(x)k(x)dx \quad D_1 \subset D \end{aligned} \quad (141)$$

Taking the integrals between the zeros we have

$$\begin{aligned} \int_{D_1} f(x)k(x)dx &= \int_0^{\xi_0} f(x)k(x)dx + \sum_{i=0}^{n-1} \int_{\xi_i}^{\xi_{i+1}} f(x)k(x)dx \\ &= \sum_{i=0}^m h_i f\left(\frac{i\xi_0}{m}\right) k\left(\frac{i\xi_0}{m}\right) + \sum_{i=0}^{n-1} h_i \sum_{j=0}^{n_i} f(\xi_i + jh_i)k(\xi_i + jh_i) \\ &= A_0 + \sum_{i=0}^{n-1} h_i \sum_{j=0}^{n_i} f(\xi_i + jh_i)k(\xi_i + jh_i) \end{aligned} \quad (142)$$

where, A_0 is the area between zero and ξ_0 , see Figure (4.1).

$$h = \frac{\xi_0 - 0}{m}, \quad h_i = \frac{\xi_{i+1} - \xi_i}{n_i} \quad ; \quad i = 0, 1, \dots, n-1 \quad (143)$$

ξ_i 's are the zeros of the integrand in question ; m is the number of quadrature points in the interval $[0, \xi_0]$; n_i is the number of quadrature points in each of the intervals $[\xi_i, \xi_{i+1}]$, $i = 0, 1, \dots, n - 1$. ¹.In the next Section we present numerical examples to validate our numerical quadrature technique.

4.2.2 Numerical experiments

For the MATLAB code, see Appendix B

For our numerical experiment, we present two examples and their numerical results. All computations are performed in MATLAB (version 7.3.0) running on Windows 2003.

Example (4.2.2.1) Let us consider the numerical quadrature for the following integral using (142)

$$I(f, g) = \int_0^{\infty} \frac{e^{-\frac{1}{2}x^2} \cos(4x)}{x^2 + 16} dx$$

Analytical result as obtained by [24] is as follows:

$$I(f, g) = \frac{\pi}{16} e^8 (2 \cosh 16 - e^{16} \operatorname{erf} \sqrt{32}) = \mathbf{0.0000723391341}$$

Our Method : **0.0000723391341**

Okecha : **0.0000723391331**

Patterson : **0.0000723391321**

Example (4.2.2.2) $I(f, g) = \int_0^{\infty} J_0(x) e^{-x} dx = \frac{1}{\sqrt{2}} = \mathbf{0.707106781186547}$

Our Method : **0.707106781186615**

¹'' denotes that the first and the last terms should be halved

4.3 Euler's transformation

In computing the value of an integral whose integrand oscillates over $[0, \infty)$, it may be useful to compute the positive and negative contributions individually and to sum the resulting infinite series, for example integrals of the form:

$$I(f, p) = \int_0^{\infty} f(x)e^{ipx} dx \quad ; p \gg 1 ; i = \sqrt{-1} \quad (144)$$

have this characteristic. This series, however, may be slowly convergent. Our next method is based on Euler's transformation of slowly convergent alternating series.

The formal transformation is most expeditiously derived by means of the calculus of finite differences, as follows:

Let

$$\Delta V_0 = V_1 - V_0 ; \Delta^2 V_0 = \Delta(\Delta V_0) = \Delta(V_1 - V_0) = V_2 - 2V_1 + V_0 ; \text{ etc} \quad (145)$$

Let

$$EV_0 = V_1 ; E^2 V_0 = V_2 ; \text{ etc} \quad (146)$$

We thus have,

$$E = \Delta + I \quad (147)$$

where I is the identity operator and Δ is the forward difference operator. Then with these operators we may write:

$$\begin{aligned}
V_0 - V_1 + V_2 - \dots &= V_0 - EV_0 + E^2V_0 - E^3V_0 + \dots \\
&= (I - E + E^2 - \dots)V_0 \\
&= (I + E)^{-1}V_0 \\
&= (2I + E - I)^{-1}V_0 \\
&= (2I + \Delta)^{-1}V_0 \\
&= \frac{1}{2}(I + \frac{1}{2}\Delta)^{-1}V_0 \\
&= \frac{1}{2}V_0 - \frac{1}{4}\Delta V_0 + \frac{1}{8}\Delta^2V_0 - \dots
\end{aligned} \tag{148}$$

where

$$V_k > 0 ; V_k > V_{k+1} \quad \forall \quad k = 0, 1, 2, \dots \tag{149}$$

It can be proved that if the left-hand series is convergent, the right-hand series is also convergent and to the same value. In numerous cases of practical interest, the right-hand series will converge more rapidly than the left-hand series.

Given the series in equation (148), it is not always desirable to start the transformation with V_0 but with some later term, say V_m , so that :

$$\sum_{k=0}^{\infty} (-1)^k V_k = \sum_{k=0}^{m-1} (-1)^k V_k + (-1)^m \left[\frac{1}{2}V_m - \frac{1}{4}\Delta V_m + \frac{1}{8}\Delta^2V_m - \dots \right] \tag{150}$$

and

$$V_k > 0 ; V_k > V_{k+1} \quad \forall \quad k = 0, 1, 2, \dots \quad (151).$$

4.3.1 Formulation of the method

Consider the integral:

$$I(f, p) = \int_0^{\infty} f(x) e^{ipx} dx \quad ; \quad p \gg 1 ; i = \sqrt{-1} \quad (152)$$

where

$f(x)$ is monotonically decreasing in $[0, \infty)$.

Without any loss of generality, let us consider the imaginary part of the integral, that is

$$\begin{aligned} I_1(f, p) &= \int_0^{\infty} f(x) \sin px \, dx \\ &= \sum_{k=0}^{\infty} \int_{\frac{k\pi}{p}}^{\frac{(k+1)\pi}{p}} f(x) \sin px \, dx \quad ; \quad k = 0, 1, \dots \\ \text{Let, } z &= x - \frac{k\pi}{p}; \end{aligned}$$

Then,

$$\begin{aligned}
I_1(f, p) &= \sum_{k=0}^{\infty} \int_0^{\frac{\pi}{p}} f\left(z + \frac{k\pi}{p}\right) \sin p\left(z + \frac{k\pi}{p}\right) dz \\
&= \sum_{k=0}^{\infty} (-1)^k \int_0^{\frac{\pi}{p}} f\left(z + \frac{k\pi}{p}\right) \sin pz dz \\
&= \sum_{k=0}^{\infty} (-1)^k V_k \quad ; \tag{153}
\end{aligned}$$

where

$$V_k = \int_0^{\frac{\pi}{p}} f\left(z + \frac{k\pi}{p}\right) \sin pz dz \tag{154}$$

Similarly, let us consider the real part of the integral

$$\begin{aligned}
I_2(f, p) &= \int_0^{\infty} f(x) \cos px dx \\
&= \int_0^{\frac{\pi}{2p}} f(x) \cos px dx + \sum_{k=0}^{\infty} \int_{\frac{(2k+1)\pi}{2p}}^{\frac{(2k+3)\pi}{2p}} f(x) \cos px dx \quad ; k = 0, 1, 2, \dots \tag{155}
\end{aligned}$$

Let,

$$z = x - \frac{(2k+1)\pi}{2p} \tag{156}$$

Then,

$$\begin{aligned}
I_2(f, p) &= \int_0^{\frac{\pi}{2p}} f(x) \cos px \, dx + \sum_{k=0}^{\infty} \int_0^{\frac{\pi}{p}} f\left(z + \frac{(2k+1)\pi}{2p}\right) \cos p\left(z + \frac{(2k+1)\pi}{2p}\right) \, dz \\
&= \int_0^{\frac{\pi}{2p}} f(x) \cos px \, dx + \sum_{k=0}^{\infty} (-1)^{k+1} \int_0^{\frac{\pi}{p}} f\left(z + \frac{(2k+1)\pi}{2p}\right) \sin pz \, dz \\
&= Q + \sum_{k=0}^{\infty} (-1)^{k+1} V_k \tag{157}
\end{aligned}$$

where

$$Q = \int_0^{\frac{\pi}{2p}} f(x) \cos px \, dx$$

and

$$V_k = \int_0^{\frac{\pi}{p}} f\left(z + \frac{(2k+1)\pi}{2p}\right) \sin pz \, dz$$

In the next Section we present numerical examples to validate our numerical quadrature technique.

4.3.2 Numerical experiments

For MATLAB code see Appendix B

Example (4.3.1.1) As test examples, we consider the following integrals,

$$I = \int_0^{\infty} e^{-x} \sin 40x \, dx = \frac{40}{1 + 40^2} \approx 0.024984$$

For this integral, we use equation (153) to generate the following table of V'_k 's.

k	V_k	ΔV_k	$10^{-3} \times \Delta^2 V_k$	$10^{-4} \times \Delta^3 V_k$	$10^{-4} \times \Delta^4 V_k$	$10^{-4} \times \Delta^5 V_k$	$10^{-4} \times \Delta^6 V_k$
0	0.048081						
1	0.044450	<u>-0.003631</u>	<u>0.273</u>				
2	0.041092	-0.003358	0.254	<u>-0.19</u>	<u>0</u>		
3	0.037988	-0.003104	0.235	-0.19	0	<u>0</u>	<u>-0.04</u>
4	0.035119	-0.002869	0.216	-0.19	-0.04	0.04	0.01
5	0.032466	-0.002653	0.201	-0.15	0.01	0.05	
6	0.030014	-0.002452	0.185	-0.16			
7	0.027747	-0.002267					

Table 4.1 First difference table for V'_k 's

$$\begin{aligned}
 \tilde{I} &= \frac{1}{2}(0.048081) - \frac{1}{4}(-0.003631) + \frac{1}{8}(0.273 \times 10^{-3}) - \frac{1}{16}(-0.19 \times 10^{-4}) + \frac{1}{32}(0) \\
 &\quad - \frac{1}{64}(0) + \frac{1}{128}(-0.04 \times 10^{-4}) - \frac{1}{256}(0.05 \times 10^{-4}) \\
 &= \mathbf{0.024984}
 \end{aligned}$$

And this is our approximate value of the integral using Euler's transformation tech-

N	ω	Our Method	Exact
50	5	0.192240	0.192308
50	40	0.024976	0.024984
100	40	0.024982	0.024984
1000	40	0.024984	0.024984

Table 4.2 First numerical results for Euler's method

nique.

Example (4.3.1.2) Similarly, consider the following integral

$$I = \int_0^{\infty} \frac{\cos 5x}{1+x^2} dx = 0.010584$$

For this integral, we use equation (157) to generate the following table of V'_k 's.

k	V_k	ΔV_k	$\Delta^2 V_k$	$\Delta^3 V_k$	$\Delta^4 V_k$	$\Delta^5 V_k$	$\Delta^6 V_k$	$\Delta^7 V_k$
0	<u>0.287052</u>							
1	0.156646	<u>-0.130406</u>						
2	0.088585	-	<u>0.062345</u>					
3	0.054992	-0.068061	0.034468	<u>-0.027877</u>				
4	0.036952	-0.033593	0.015530	-0.018915	<u>0.008962</u>			
5	0.063730	-0.018040	0.007461	-0.008092	0.010823	<u>0.001861</u>		
6	0.019704	-0.010579	0.003910	-0.003551	0.004541	-0.006282	<u>-0.008143</u>	
7	0.015253	-0.006669	0.002218	-0.001692	0.001859	-0.002682	0.003600	<u>0.011743</u>
		-0.004451						

Table 4.3 Second difference table for V'_k 's

$$\tilde{I} = Q + \sum_{k=0}^{m-1} (-1)^k V_k + (-1)^m \left[\frac{1}{2} V_m - \frac{1}{4} \Delta V_m + \frac{1}{8} \Delta^2 V_m - \dots \right]$$

$$\begin{aligned} \tilde{I} &= 0.19638790 - \left[\frac{1}{2}(0.287052) - \frac{1}{4}(-0.130406) + \frac{1}{8}(0.062345) - \frac{1}{16}(-0.027877) + \frac{1}{32}(0.008962) \right. \\ &\quad \left. - \frac{1}{64}(0.001861) + \frac{1}{128}(-0.008143) - \frac{1}{256}(0.011743) \right] \\ &= \mathbf{0.010584} \end{aligned}$$

This is our approximate value of the integral using Euler's transformation technique.

Results for $I = \int_0^{\infty} \frac{\cos \omega x}{1+x^2} dx$

N	ω	Our Method	Exact
45	5	0.010584	0.010584
393	10	7.13142×10^{-5}	7.13140×10^{-5}

Table 4.4 Second numerical results for Euler's method

CHAPTER 5. Collocation method with Applications

In this Section we present a method wherein the smooth function of the integrand is replaced with a truncated Chebyshev series approximation and the unknown Chebyshev coefficients are evaluated by a collocation method. The resulting moments are evaluated using the methods due to Piessens et al [28] and Levin [18]. Some examples have been presented to illustrate the method.

If ω is a very small positive real constant on a finite interval (a, b) and if $f(x)$ is sufficiently smooth in (a, b) , then it is well known that the integrals of the form

$$I(f, \omega) = \int_a^b f(x)e^{i\omega x} dx, \quad x \in (a, b) \quad (161)$$

can be evaluated numerically by Gaussian quadrature rules. However, if the magnitude of ω becomes very large and $f(x)$ decreases slowly, then the problem of numerical computation of these integrals becomes considerably more difficult. In this Section we shall present a quadrature formula for the evaluation of integral (161) above. We shall assume throughout this Section that $f(x)$ is smooth and $e^{i\omega x}$ is highly oscillatory in $[a, b]$. In this paper the problem of computing the integral is transformed into a problem of finding a solution of a linear system with the zeros of a Chebyshev polynomial as collocation points and the resulting moments are evaluated using the methods due to Piessens et al [28] and Levin [18].

5.1 Approximation Theory of Chebyshev series [4]

Suppose we want to compute

$$F(x) = \int_a^x f(t)dt ; a \leq x \leq b \quad (162)$$

for a given integrand $f(x)$ which is analytic in $[a, b]$.

Suppose further, that we have an approximation to $f(x)$ of the form:

$$f(x) = \sum_{i=0}^n a_i \phi_i(x) + \epsilon(x) ; a \leq x \leq b \quad (163)$$

where

$$|\epsilon(x)| \leq \epsilon , a \leq x \leq b$$

and where each of the approximating functions ϕ_i has an indefinite integral

$$\psi_i(x) = \int_a^x \phi_i(t)dt \quad (164)$$

which is simple to handle, then integrating (163) we obtain

$$F(x) = \int_a^x f(t)dt = \sum_{i=0}^n a_i \psi_i(x) + \eta(x) \quad (165)$$

where

$$|\eta(x)| = \left| \int_a^x \epsilon(t) dt \right| \leq (b - a) \epsilon \quad (166)$$

In principle, we may employ any sort of approximating form of (163), but in practice it turns out to be particularly convenient to use expansions in terms of orthogonal polynomials, especially the Chebyshev polynomials $T_n(x)$.

It can be shown that if $f(x)$ is of class $C^\infty[-1, 1]$, then $f(x)$ may be expanded in a uniformly convergent series of Chebyshev polynomials:

$$f(x) = \frac{1}{2}\alpha_0 + \sum_{i=1}^{\infty} \alpha_i T_i(x) \quad (167)$$

The constants α_i are the Fourier Chebyshev coefficients of $f(x)$ and are given by the formula

$$\alpha_i = \frac{2}{\pi} \int_{-1}^1 \frac{f(x)T_i(x)}{\sqrt{1-x^2}} dx = \frac{2}{\pi} \int_0^\pi f(\cos(\theta)) \cos(i\theta) d\theta \quad (168)$$

For many functions the sequence $\alpha_0, \alpha_1, \dots$ decreases to zero rapidly. Furthermore, the partial sum

$$f(x) = \frac{1}{2}\alpha_0 + \sum_{i=1}^N \alpha_i T_i(x) \quad (169)$$

is a polynomial of degree $\leq N$, which is very close to the best approximation to $f(x)$ by polynomials $P_N(x)$ of this degree, approximation being measured in the sense of

$$\max_{-1 \leq x \leq 1} |f(x) - P_N(x)|$$

In any case, we have the estimate

$$\begin{aligned} \left| f(x) - \sum_{i=0}^N \alpha_i T_i(x) \right| &= \left| \sum_{i=N+1}^{\infty} \alpha_i T_i(x) \right| \\ &\leq \sum_{i=N+1}^{\infty} |\alpha_i|, \quad -1 \leq x \leq 1 \end{aligned} \quad (170)$$

In general, the coefficients α_i may not be obtained in a closed form, therefore one must seek an approximation to them. One may apply trapezoidal rule for instance.

If we integrate the uniformly convergent series in (169) term by term, we obtain

$$\begin{aligned} \int f(x) dx &= \frac{\alpha_0}{2} T_1(x) + \frac{\alpha_1}{4} T_2(x) + \sum_{i=2}^{\infty} \frac{\alpha_i}{2} \left(\frac{T_{i+1}(x)}{i+1} - \frac{T_{i-1}(x)}{i-1} \right) + \text{constant} \\ &= \sum_{i=0}^{\infty} A_i T_i(x) \end{aligned} \quad (171)$$

where

$$A_i = \frac{\alpha_{i-1} - \alpha_{i+1}}{2i}, \quad i > 0$$

The constant A_0 should be selected so that the indefinite integral is zero at the lower limit of integration.

5.2 Description of method

5.2.1 Collocation scheme

Our aim is to find a suitable approximation to the integral of the form:

$$I(f, \omega) = \int_a^b f(x)e^{i\omega x} dx \quad , \quad x \in (a, b) \quad , \quad \text{where } \omega \gg 1 \quad (172)$$

Without any loss of generality we now replace the arbitrary interval (a, b) with the interval $[-1, 1]$.

If we substitute equation (169) into equation (172) we obtain

$$I(f, \omega) = \int_{-1}^1 \sum_{r=0}^{\infty} \alpha_r T_r(x) e^{i\omega x} dx = \sum_{r=0}^{\infty} \alpha_r \int_{-1}^1 T_r(x) e^{i\omega x} dx \quad (173)$$

The Fourier Chebyshev coefficients α_r usually decrease to zero rapidly, and this phenomenon has led to the use of a truncated version of equation (167) in practice, which is equation (169) and this leads to

$$\begin{aligned} I(f, \omega) &\approx \int_{-1}^1 \sum_{r=0}^N \alpha_r T_r(x) e^{i\omega x} dx \\ &= \sum_{r=0}^N \alpha_r \int_{-1}^1 T_r(x) e^{i\omega x} dx \\ &= \sum_{r=0}^N \alpha_r \gamma_r \end{aligned} \quad (174)$$

where

$$\gamma_r = \int_{-1}^1 T_r(x) e^{i\omega x} dx \quad (175)$$

5.2.2 Evaluation of α_r

Consider equation (169), which is

$$f(x) = \sum_{r=0}^N \alpha_r T_r(x) \quad (176)$$

This is a linear combination of Chebyshev polynomials and the moments α_r 's, if we collocate at the points $\{x_i\}_{i=1}^{N+1} \subset (-1, 1)$, then we can conveniently express (176) in matrix form

$$\mathbf{T} \boldsymbol{\alpha} = \mathbf{F} \quad (177)$$

where

$$\mathbf{T} = \begin{bmatrix} T_0(x_1) & T_1(x_1) & \dots & T_N(x_1) \\ T_0(x_2) & T_1(x_2) & \dots & T_N(x_2) \\ \vdots & \vdots & \dots & \vdots \\ T_0(x_N) & T_1(x_N) & \dots & T_N(x_N) \\ T_0(x_{N+1}) & T_1(x_{N+1}) & \dots & T_N(x_{N+1}) \end{bmatrix}$$

$$\begin{aligned}\mathbf{F} &= [f(x_1), f(x_2), \dots, f(x_N), f(x_{N+1})]^T \\ \alpha &= [\alpha_0, \alpha_1, \dots, \alpha_{N-1}, \alpha_N]^T\end{aligned}$$

where

$$x_j = \cos\left(\frac{2j-1}{2(N+1)}\pi\right), \quad j = 1, \dots, N+1.$$

which are the zeros of $T_{N+1}(x)$

This linear system may be solved using Cramer's rule or by the inverse matrix method, and the latter yields to the form

$$\alpha = \mathbf{T}^{-1} \mathbf{F} \quad (178)$$

The linear system may also be solved using a simple Matlab command since the matrix T is stable and invertible.

5.2.3 Evaluation of γ_r Method 1 see [18]

The Levin Collocation Method [18], approximates oscillatory integrals without stationary points and without any moments.

Consider the integral

$$\gamma_r = \int_{-1}^1 T_r(x) e^{i\omega x} dx, \quad x \in (-1, 1) \quad (179)$$

he seeks a function $F_r(x)$ such that

$$\frac{d}{dx} [F_r(x) e^{i\omega x}] = [F_r'(x) + i\omega F_r(x)] e^{i\omega x} = T_r(x) e^{i\omega x} \quad (180)$$

so that

$$\gamma_r = \int_{-1}^1 T_r(x) e^{i\omega x} dx = \int_{-1}^1 \frac{d}{dx} [F_r(x) e^{i\omega x}] dx = F_r(1) e^{i\omega(1)} - F_r(-1) e^{i\omega(-1)} \quad (181)$$

Levin proposed an approximation to $F_r(x)$ of the form

$$F_r(x) \approx \tilde{F}_r(x) = \sum_{k=0}^N a_{rk} \psi_k(x) \quad (182)$$

where $\{\psi_k\}_{k=0}^N$ are linearly-independent basis functions.

In our case we choose the bases functions to be the Chebyshev polynomials and collocate the equation

$$\sum_{k=0}^N [T'_k(x_j) + i\omega T_k(x_j)] a_{rk} = T_r(x_j); \quad j = 1, 2, \dots, N+1; \quad \text{for each } \gamma_r \quad (183)$$

Equation (183) is a linear system of the form

$$\tilde{T} A_r = T_r \quad (184)$$

where

$$A_r = [a_{r0}, a_{r1}, \dots, a_{rN}]^T$$

$$\tilde{T} = \begin{bmatrix} T'_0(x_1) + i\omega T_0(x_1) & T'_1(x_1) + i\omega T_1(x_1) & \dots & T'_N(x_1) + i\omega T_N(x_1) \\ T'_0(x_2) + i\omega T_0(x_2) & T'_1(x_2) + i\omega T_1(x_2) & \dots & T'_N(x_2) + i\omega T_N(x_2) \\ \vdots & \vdots & \dots & \vdots \\ T'_0(x_N) + i\omega T_0(x_N) & T'_1(x_N) + i\omega T_1(x_N) & \dots & T'_N(x_N) + i\omega T_N(x_N) \\ T'_0(x_{N+1}) + i\omega T_0(x_{N+1}) & T'_1(x_{N+1}) + i\omega T_1(x_{N+1}) & \dots & T'_N(x_{N+1}) + i\omega T_N(x_{N+1}) \end{bmatrix}$$

$$T_r = [T_r(x_1), T_r(x_2), \dots, T_r(x_N), T_r(x_{N+1})]^T$$

where

$$x_j = \cos\left(\frac{2j-1}{2(N+1)}\pi\right), \quad j = 1, \dots, N+1.$$

which are the zeros of $T_{N+1}(x)$

This linear system is solved by the inverse matrix method, and this yields to the form

$$A_r = \tilde{T}^{-1} T_r \tag{185}$$

and this may also be solved using a simple Matlab command since the matrix \tilde{F} is stable and invertible.

Thus,

$$\gamma_r = \int_{-1}^1 T_r(x) e^{i\omega x} dx \approx \tilde{F}_r(1) e^{i\omega(1)} - \tilde{F}_r(-1) e^{i\omega(-1)} \quad (186)$$

5.2.4 Evaluation of γ_r Method 2 see[29]

Piessens and Poleunis [29] developed the following method for the integration of Fourier coefficients which they claim gives high accuracy at low cost.

The idea is to use the relations

$$\int_{-1}^1 \frac{\sin(mx) T_n(x)}{\sqrt{(1-x^2)}} dx = \begin{cases} 0 & , n = 2k \\ (-1)^k \pi J_n(m) & , n = 2k + 1 \end{cases} \quad (187)$$

$$\int_{-1}^1 \frac{\cos(mx) T_n(x)}{\sqrt{(1-x^2)}} dx = \begin{cases} (-1)^k \pi J_n(m) & , n = 2k \\ 0 & , n = 2k + 1 \end{cases} \quad (188)$$

If we then have the expansion

$$\sqrt{(1-x^2)} f(x) = \sum_{n=0}^{\infty} 'C_n T_n(x)$$

We then have

$$S(m) = \int_{-1}^1 f(x) \sin(mx) dx = \pi \sum_{k=0}^{\infty} C_{2k+1} (-1)^k J_{2k+1}(m) \quad (189)$$

$$C(m) = \int_{-1}^1 f(x) \cos(mx) dx = \pi \sum_{k=0}^{\infty} 'C_{2k} (-1)^k J_{2k}(m) \quad (190)$$

J_n 's are the Bessel functions of the first kind and order n .

The C_n 's are approximated by the following formulas

$$C_{2k} \approx \frac{-2}{\pi} \sum_{i=0}^{[N/2]} \alpha_{2i} \left[\frac{1}{(2i+2k)^2-1} + \frac{1}{(2i-2k)^2-1} \right] \quad (191)$$

$$C_{2k+1} \approx \frac{-2}{\pi} \sum_{i=0}^{[(N-1)/2]} \alpha_{2i+1} \left[\frac{1}{(2i+2k+2)^2-1} + \frac{1}{(2i-2k)^2-1} \right] \quad (192)$$

where N is chosen to be sufficiently large.

In a paper by Piessens and Branders [28], the following recurrence relations have also been established to evaluate γ_r .

$$\text{Re}(\gamma_r(x)) = I_r(x) = \int_{-1}^1 T_r(x) \cos(\omega x) dx.$$

The three term non-homogeneous recurrence relation is

$$\begin{aligned} 24\omega \sin \omega - 8(r^2 - 4) \cos \omega &= \omega^2(r-1)I_{r+2} - 2(r^2-4)(\omega^2 - 2r^2 + 2)I_r \\ &+ \omega^2(r+1)(r+2)I_{r-2} \end{aligned}$$

with starting values

$$\begin{aligned} I_0 &= \frac{2 \sin \omega}{\omega} \\ I_2 &= \frac{8 \cos \omega}{\omega^2} + \frac{(2\omega^2 - 8) \sin \omega}{\omega^3} \\ I_4 &= \frac{32(\omega^2 - 12) \cos \omega}{\omega^4} + \frac{2(\omega^4 - 80\omega^2 + 192) \sin \omega}{\omega^5} \end{aligned}$$

and the forward recursion is numerically stable up to $r = |\omega|$ but beyond this, one may use the backward recursion algorithm. $I_r = 0$ for r odd.

Similarly, in [28]

$$\text{Im}(\gamma_r(x)) = I_r(x) = \int_{-1}^1 T_r(x) \sin(\omega x) dx$$

and we have the recursion equation

$$\begin{aligned} -24\omega \cos \omega - 8(r^2 - 4) \sin \omega &= \omega^2(r - 1)I_{r+2} - 2(r^2 - 4)(\omega^2 - 2r^2 + 2)I_r \\ &+ \omega^2(r + 1)(r + 2)I_{r-2} \end{aligned}$$

with starting values

$$\begin{aligned} I_1 &= 2 \frac{(\sin \omega - \omega \cos \omega)}{\omega^2} \\ I_3 &= \left(18 - \frac{48}{\omega^2}\right) \frac{\sin \omega}{\omega^2} + \left(\left(\frac{48}{\omega^2} - 2\right) \frac{\cos \omega}{\omega}\right) \end{aligned}$$

$I_r = 0$ when r is even.

The stability problem is same as in the preceding case. In the next section we present numerical examples to give credence to our quadrature scheme and compare with some well known numerical integration methods. In our numerical examples we will use the preceding results to evaluate the oscillatory moments

$$\gamma_r = \int_{-1}^1 T_r(x) e^{i\omega x} dx \quad (193)$$

Here we use the fact that

$$\int_{-1}^1 T_n(x) \sin(\omega x) dx = \begin{cases} 0 & \text{if } n \text{ is even} \\ \pi \sum_{k=0}^{\infty} C_{2k+1} (-1)^k J_{2k+1}(\omega) & \text{if } n \text{ is odd} \end{cases} \quad (194)$$

$$\int_{-1}^1 T_n(x) \cos(\omega x) dx = \begin{cases} 0 & \text{if } n \text{ is odd} \\ \pi \sum_{k=0}^{\infty} C_{2k} (-1)^k J_{2k}(\omega) & \text{if } n \text{ is even} \end{cases} \quad (195)$$

Both series are convergent and the terms decrease with increasing k and $k > \frac{\omega}{2}$. The errors in $S(m)$ and $C(m)$, which we call R_s and R_c respectively, according to Kythe et al[3] are

$$R_s \approx -2 \sin \omega \sum_{k=[\frac{N+1}{2}]}^{\infty} \frac{\alpha_{2k+1}}{(2k+1)^2}$$

$$R_c \approx -\frac{\cos \omega}{2} \sum_{k=[\frac{N}{2}+1]}^{\infty} \frac{\alpha_{2k}}{(k)^2}$$

Therefore, as $k \rightarrow \infty$ the quadrature formulae (189) and (190) converge very fast, even faster than the Chebyshev series for $f(x)$.

5.3 Numerical experiments

For MATLAB code see Appendix C

Example (5.3.1) We use **Method 1** to solve numerically the integral

$$I = \int_{-1}^1 \cos \frac{\pi}{4} t^2 \cos \frac{\pi}{4} 41t \, dt$$

$$\text{exact} = 0.02966470953267$$

$$\text{approx} = 0.02966470956820$$

Example (5.3.2) We use the integral that was considered by H.V. Smith[31] and Piessens and Poleunis[29], to illustrate our quadrature scheme.

$$I(f, \omega) = \int_{-1}^1 \frac{\sin(\omega x)}{x + 3} dx$$

From equation (194) we use only the first eight terms to evaluate our moments γ_r and equation (174) with $N = 14$ to evaluate α_r and the results are given in **Table 1** below.

r	α_{2r+1}	γ_{2r+1}
0	-0.121320343559643	0.156940522405102
1	-0.003571337468205	0.032233604311279
2	-0.000105130359325	-0.318289405748126
3	-0.000003094748830	-0.448106145005634
4	-0.000000091100900	0.842566000282360
5	-0.000000002681760	-0.414144522152262
6	-0.000000000078942	0.110954443265098
7	-0.000000000002255	0.110954443265099

Table 5.1 α and γ for $\omega = 10$

From (174) and Table 5.1, working within six decimal digits, we obtain

$$I(f, \omega) = \int_{-1}^1 \frac{\sin(10x)}{x+3} dx$$

exact = -0.019120

approx = -0.019120

In Table 5.2, we compare our results with some known results for different values of ω .

ω	Exact	Piessens et al (N = 4)	H.V. Smith (N = 5)	<i>Our results for (N=5)</i>	
				Method2	Method 1
1	-0.071675	-0.071682	-0.071675	-0.071675	-0.071675
2	-0.103085	-0.103102	-0.103085	-0.103085	-0.103085
4	-0.025117	-0.025132	-0.025117	-0.025117	-0.025117
10	-0.019120	-0.019140	-0.019122	-0.019122	-0.019121

Table 5.2 Numerical Results for collocation method

CHAPTER 6. Conclusion and pointers for future work

In this research we successfully demonstrated the application of the Gauss Legendre quadrature scheme with some modifications of course. This was shown with the numerical experiments involving Cauchy type integrals, and the results are quite comparable to the results obtained by several renowned authors in this field. The problem of high oscillation has been addressed by using the classical composite trapezoidal rule and integration between the zeros. And lastly we have demonstrated the successful numerical integration of oscillatory integrals without any need for the oscillatory moments evaluation as this is sometimes very laborious.

The challenges of numerical integration have so far evolved around one dimensional integrals and very little research output has been published in multi dimensional cases. This area will need much more attention in future as technological innovations demand very innovative thinking in any mathematical field. Emphasis needs to be put on the exact error prediction for each approximate rule. The error formulas are not yet that simple to apply and there could be some improvement in this field if we numerical scientists could focus more on deriving the exact error formulas.

APPENDIX A. MATLAB codes for Chapter Three

Finding the zeros of a Legendre polynomial of the first kind

```
n=the order of  $P_n(t)$ ;  
 $J = \text{zeros}(n)$ ;  
for  $i = 1 : n$   
 $J(i, i) = 0$ ;  
for  $j = 2 : n$   
 $J(j, j - 1) = \text{sqrt}((j - 1).^2 ./ (4 * (j - 1).^2 - 1))$ ;  
 $J(j - 1, j) = J(j, j - 1)$ ;  
end  
end  
 $[V, D] = \text{eig}(J)$ 
```

Code for Example 3.5.1

```
 $f = \text{inline}('(\text{exp}(-0.5 * x) - \text{exp}(-0.25 * -0.5)) / (x + 0.25)')$ ;  
 $f1 = \text{inline}(' \text{exp}(-0.5 * x)')$ ;  
  
 $t = [0.9061798459 - 0.90617984590.5384693101 - 0.53846931010]$ ; define zeros  
 $w = [0.23692688510.23692688510.47862867050.47862867050.5688888888]$ ; define weights
```

```

sum = 0;
for i = 1 : 5
G(i) = w(i) .* f(t(i));
sum = sum + G(i);
I2 = sum;
end
I = exp(-0.5) .* I2 + exp(-0.5) .* f1(-0.25) .* log((1 + 0.25)/(1 - 0.25))

```

Code for Example 3.5.2

```

g = inline('( (25 - x.^2).^(-0.5) - (25 - (0.5)^2).^(-0.5) ) ./ (x - 0.5)');
g1 = inline('1/(x * (x + 0.5))');
f = inline('(25 - x.^2).^(-0.5)');
P0 = 1;
P1 = inline('x');
P2 = inline('(3 * x.^2 - 1)/2');
P3 = inline('(5 * x.^3 - 3 * x)/2');
P5 = inline('(63 * x.^5 - 70 * x.^3 + 15 * x)/8');
P6 = inline('(231 * x.^6 - 315 * x.^4 + 105 * x.^2 - 5)/16');

Q0 = inline('0.5 * log((1 + x)/(1 - x))');
Q1 = inline('0.5 * x * log((1 + x)/(1 - x)) - 1');
Q2 = inline('(3 * x^2 - 1)/4 * log((1 + x)/(1 - x)) - (3 * x/2)');
Q3 = inline('(5 * x^3 - 3 * x)/4 * log((1 + x)/(1 - x)) - 5 * x^2/2 + (2/3)');
Q4 = inline('(1/16) * (35 * x.^4 - 30 * x.^2 + 3) * log((1 + x)/(1 - x)) - (35 * x.^3/8) + (55 * x/24)');
Q5 = inline('(1/16) * (63 * x.^5 - 70 * x.^3 + 15 * x) * log((1 + x)/(1 - x)) - (63 * x.^4/8) +

```

```

(49 * x.^2/8) - (8/15)');
; I8 = 2 * f(0.5)/ - 0.75;
t = [0.9324695142 - 0.9324695142 0.6612093865 - 0.6612093865 0.2386191861 -
0.2386191861];
w = [0.1713244924 0.1713244924 0.3607615730 0.3607615730 0.4679139346 0.4679139346];
sum = 0;
for j = 1 : 6

```

$$\begin{aligned}
A(j) = & w(j) \cdot (g(t(j)) \cdot P0 \cdot Q0(0.5) + g(t(j)) \cdot P1(t(j)) \cdot Q1(0.5) \cdot 3 \\
& + g(t(j)) \cdot P2(t(j)) \cdot Q2(0.5) \cdot 5 + g(t(j)) \cdot P3(t(j)) \cdot Q3(0.5) \cdot 7 \\
& + g(t(j)) \cdot P4(t(j)) \cdot Q4(0.5) \cdot 9 + g(t(j)) \cdot P5(t(j)) \cdot Q5(0.5) \cdot 11);
\end{aligned}$$

```

sum = sum + A(j);
II = sum;
end
Answer = I8 - II

```

APPENDIX B. MATLAB codes for Chapter Four

Matlab code for Example 4.2.2.1

```
for n = 1 : 128
p(n) = (2 * n + 1) .* (pi/8);
end
sum = 0;
for n = 1 : 10
xn = p(n) : 0.000001 : p(n + 1);
X = (exp(-0.5 * xn.^2) .* cos(4 * xn))./(xn.^2 + 16);
Y(n) = trapz(xn, X);
sum = sum + Y(n);
Ans2 = sum;
end

x=0:0.000001:p(1);Integration of the area between zero and the first zero
. Z=(exp((-0.5)*x.^2) .* cos(4 * x))./(x.^2 + 16);
A = trapz(x, Z);
Approx = Ans2 + A;
exact = ((pi/16) * exp(8)) .* (2 * cosh(16) - (exp(16) * erf(sqrt(32))));
error = abs(exact - Approx);
```

Matlab code for Example 4.2.2.2

```
bessj0=inline('besselj(0,t)');

for n=1:100
z(n)=fzero(bessj0,[(n-1) n]*pi);
end
sum = 0;
for n=1:9
tn=(z(n):0.000001:z(n+1))';
Z=besselj(0,tn).*exp(-(tn));
K(n)=trapz(tn,Z);
sum=sum + K(n);
Ans = sum;
end
```

```
t=0:0.000001:z(1);Integration of the area between zero and the first zero
. P=besselj(0,t).*exp(-t);
Q=trapz(t,P);
Appr=Q+Ans;
ex=1/sqrt(2);
Er=abs(ex-Appr);
```

Matlab code for Example 4.3.1.1

```
p = 40;
a=0 ; b=pi/p;
```

```

N=1000; h=(b-a)/N;
for k = 1:8
sum = 0;
for j = 1:N+1
x(j) = a + (j-1)*h;
P(j) = exp(-(x(j)+(k-1)*pi/p)).*sin(p*x(j));
if j==1—j==N+1
P(j) = 0.5*P(j);
end
sum = sum + P(j);
A(k) = h*sum;
end

end

for i = 2:8
B(i-1)=A(i)-A(i-1);
end

for i = 2:7
C(i-1)=B(i)-B(i-1);
end

for i = 2:6
D(i-1)=C(i)-C(i-1);
end

for i = 2:5
E(i-1)=D(i)-D(i-1);
end

for i = 2:4

```

```
F(i-1)=E(i)-E(i-1);
```

```
end
```

```
for i = 2:3
```

```
G(i-1)=F(i)-F(i-1);
```

```
end
```

```
H = G(2)-G(1);
```

```
Ans = 0.5 * A(1) - (1/4) * B(1) + (1/8) * C(1) - (1/16) * D(1) + (1/32) * E(1)  
      -(1/64) * F(1) + (1/128) * G(1) - (1/256) * H;
```

Matlab code for Example 4.3.1.2

```
p = 5;
```

```
a=0 ; b=pi/p; b1=pi/(2*p);
```

```
N=45; h=(b-a)/N; h1=(b1-a)/N;
```

```
sum = 0;
```

```
E2 = exp(-p)*pi*0.5;
```

```
for k = 1:N+1
```

```
t(k) = a + (k-1)*h1;
```

```
f(k) = cos(p*t(k))./(1+(t(k)).^2);
```

```
if k == 1 | k == N + 1
```

```
f(k) = 0.5 * f(k);
```

```
end
```

```
sum = sum + f(k);
```

```
Q = h1 * sum;
```

```
end
```

```
    for k = 1:8
```

```
        sum = 0;
```

```
        for j = 1:N+1
```

```
            x(j) = a + (j-1)*h;
```

```
            P(j) = sin(p*x(j))./(1+(x(j)+((2*k-1)*pi/(2*p))).2);
```

```
            if j == 1 | j == N + 1
```

```
                P(j) = 0.5 * P(j);
```

```
            end
```

```
            sum = sum + P(j);
```

```
            A(k) = h * sum;
```

```
        end
```

```
    end
```

```
    for i = 2:8
```

```
        B(i-1) = A(i) - A(i-1);
```

```
    end
```

```
    for i = 2:7
```

```
        C(i-1) = B(i) - B(i-1);
```

```
    end
```

```
    for i = 2:6
```

```
        D(i-1) = C(i) - C(i-1);
```

```
    end
```

```
    for i = 2:5
```

$E(i-1)=D(i)-D(i-1);$

end

for i = 2:4

$F(i-1)=E(i)-E(i-1);$

end

for i = 2:3

$G(i-1)=F(i)-F(i-1);$

end

$H = G(2)-G(1);$

$$\begin{aligned} Ans1 = & Q - (0.5 * A(1) - (1/4) * B(1) + (1/8) * C(1) - (1/16) * D(1) \\ & +(1/32) * E(1) - (1/64) * F(1) + (1/128) * G(1) - (1/256) * H); \end{aligned}$$

APPENDIX C. MATLAB code for Chapter Five

Matlab code for Example 5.3.2 using method 1

```
n=15;
d=pi/(2*n);
w = 10;
C=ones(1,n);
Chebyshev polynomials
for k=1:n
for j=1:n
X(k)=cos((2*k-1)*d);
T(j,k)=cos((j-1)*acos(X(k)))*i*w+(j-1)*sin((j-1)*acos(X(k))).*(1/sqrt(1-(X(k)).^2));
Y = inline('1./(t + 3)');
P(j,k) = cos((j - 1) * acos(X(k)));
fx = Y(X);
end
end
A = zeros(n, 1);
sum = 0;
for j = 1 : n
A(:, j) = inv(T.') * P(j, :).';
P2(j) = cos((j - 1) * acos(1)) * exp(i * 10) - cos((j - 1) * acos(-1)) * exp(-i * 10);
```

```
 $g(j) = P2 * A(:, j);$  Evaluation of gammas  
end
```

```
Ap=inv(P.)*fx. '; Evaluation of alphas  
Ans = imag(Ap.*g.');
```

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