UNIVERSITI PUTRA MALAYSIA

MODIFIED SPLINE FUNCTIONS AND CHEBYSHEV POLYNOMIALS FOR THE SOLUTION OF HYPERSINGULAR INTEGRALS PROBLEMS

LAWAN SIRAJO BICHI

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By

LAWAN SIRAJO BICHI

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

December 2015

DEDICATIONS

I dedicate this work of mine to my parents Alhaji Lawan Mai-goro and late Khadijah as well as my family. May the mercy of Allah be upon us all. Your support and courage is what made me who I am today. Thank you.

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the degree of Doctor of Philosophy

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Chair: Prof. Madya. Zainidin Eshkuvatov, PhD
Faculty: Science

The research work studied the singular integration problems of the form

$$H_k(x,y)=\begin{cases}\iint\limits_{\Omega}\dfrac{h(x,y)}{|\bar{x}-\bar{x}_0^*|^{2-\gamma}}dA,\ 0\le\gamma\le 1, & k=1,\\ \iint\limits_{\Omega} h(x,y)\log|\bar{x}-\bar{x}_0^*|dA, & k=2,\end{cases}$$

where $\Omega=[a_1,a_2]\times[b_1,b_2]$, $\bar{x}=(x,y)\in\Omega$ and fixed point $\bar{x}_0^*=(x_0^*,y_0^*)\in\Omega$. The density function $h(x,y)$ is given, continuous and smooth on the rectangle Ω and belong to the class of functions $C^{2,\gamma}(\Omega)$.

Cubature formulas for double integrals with algebraic and logarithmic singularities on a rectangle Ω are constructed using the modified spline function $S_\Lambda(P)$ of type $(0,2)$. Exactness of the cubature formulas for the two cases $k\in\{1,2\}$ together with tested examples are shown each for linear and quadratic functions. Highly accurate numerical results for the cubature formulas are given for both tested density function $h(x,y)$ as linear and quadratic functions. The results are in line with the theoretical findings.

Further more, Hadamard type hypersingular integral (HSI) of the form

$$H_i(h,x)=\frac{w_i(x)}{\pi}\,=\!\!\!\!\!\!\!\int_{-1}^{1}\frac{h(t)}{w_i(t)(t-x)^2}dt,\, x\in(-1,1),\, i\in\{1,2,3,4\},$$

where $w_1(t)=\sqrt{1-t^2}$, $w_2(t)=\frac{1}{\sqrt{1-t^2}}$, $w_3(t)=\sqrt{\frac{1-t}{1+t}}$ and $w_4(t)=\sqrt{\frac{1+t}{1-t}}$ are the weights and $h(t)$ is a smooth function, are considered. Automatic quadrature schemes (AQSs) in each case for $i\in\{1,2,3,4\}$ are constructed via approximating the density function $h(t)$ by the first, second, third and fourth kind truncated series of Chebyshev polynomials, respectively. Error estimations in the cases $i\in\{1,2,3,4\}$ are obtained via approximating the density function by truncated series of Chebyshev polynomials of the first, second, third and fourth kind, respectively, in the class of function $C^{N,\alpha}[-1,1]$. Exactness of the methods each for $i\in\{1,2,3,4\}$ are shown for the degree 3 polynomial functions and the results of tested examples are presented and discussed. Numerical results of the obtained quadrature schemes revealed that the proposed methods are highly accurate for the tested density function $h(t)$ as polynomial and rational functions. Comparisons made with other known methods showed that the automatic quadrature schemes (AQSs) constructed in this research has better results than others. The results are in line with the theoretical findings.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk ijazah Doktor Falsafah

FUNGSI SPLIN TERUBAHSUAI DAN POLINOMIAL CHEBYSHEV BAGI PENYELESAIAN MASALAH KAMIRAN HIPERSINGULAR

Oleh

LAWAN SIRAJO BICHI

Disember 2015

Pengerusi: Prof. Madya. Zainidin Eshkuvatov, PhD
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Penyelidikan ini mengkaji masalah pengamiran singular dalam bentuk

$$H_k(x,y) = \begin{cases} \displaystyle\iint_{\Omega} \frac{h(x,y)}{|\bar{x}-\bar{x}_0^*|^{2-\gamma}} dA, 0 \le \gamma \le 1, & k = 1, \\ \displaystyle\iint_{\Omega} h(x,y) \log|\bar{x}-\bar{x}_0^*| dA, & k = 2, \end{cases}$$

dengan $\Omega = [a_1,a_2] \times [b_1,b_2]$, $\bar{x} = (x,y) \in \Omega$ dan titik tetap $\bar{x}_0^* = (x_0^*, y_0^*) \in \Omega$. Fungsi ketumpatan $h(x,y)$ diberi, selanjar dan mulus di atas segi empat Ω dan tergolong dalam kelas fungsi $C^{2,\gamma}(\Omega)$.

Formula pengkiuban untuk kamiran ganda dua dengan singulariti berbentuk aljabar dan logaritma di atas segiempat Ω dibina menggunakan fungsi splin terubahsuai $S_\Lambda(P)$ jenis $(0,2)$. Ketepatan formula pengkiuban untuk kedua-dua kes $k \in \{1,2\}$ bersama-sama dengan contoh teruji bagi fungsi linear dan kuadratik ditunjukkan. Keputusan berangka yang sangat tepat bagi formula pengkiuban disertakan bagi kedua-dua fungsi ketumpatan teruji $h(x,y)$ sebagai fungsi linear dan kuadratik. Keputusan yang diperolehi adalah selari dengan penemuan secara teori.

Selanjutnya, kamiran hipersingular jenis Hadamard (KHH) dalam bentuk

$$H_i(h,x) = \frac{w_i(x)}{\pi} \int_{-1}^{1} \frac{h(t)}{w_i(t)(t-x)^2} dt,\ x \in (-1,1),\ i \in \{1,2,3,4\},$$

dengan $w_1(t) = \sqrt{1-t^2}$, $w_2(t) = \frac{1}{\sqrt{1-t^2}}$, $w_3(t) = \sqrt{\frac{1-t}{1+t}}$ dan $w_4(t) = \sqrt{\frac{1+t}{1-t}}$ adalah pemberat dan $h(t)$ adalah fungsi mulus. Skim kuadratur automatik (SKA) bagi setiap kes $i \in \{1,2,3,4\}$ dibina dengan menghampirkan fungsi ketumpatan $h(t)$ dengan siri polinomial Chebyshev terpangkas jenis pertama, kedua, ketiga dan keempat. Anggaran ralat bagi kes $i \in \{1,2,3,4\}$ diperolehi dengan menghampirkan fungsi ketumpatan dengan siri polinomial chebyshev terpangkas jenis pertama, kedua, ketiga dan keempat, dalam fungsi kelas $C^{N,\alpha}[-1,1]$. Ketepatan kaedah bagi kes $i \in \{1,2,3,4\}$ dipamerkan untuk fungsi polinomial berdarjah 3 dan keputusan bagi contoh teruji dibentangkan dan dibincangkan. Keputusan berangka bagi skim kuadratur yang diperolehi mendedahkan bahawa kaedah yang dicadangkan adalah sangat tepat untuk fungsi ketumpatan teruji $h(t)$ sebagai fungsi polinomial dan fungsi nisbah. Pembandingan yang telah dibuat dengan kaedah lain yang diketahui menunjukkan bahawa skim kuadratur automatik (SKA) yang telah dibina dalam penyelidikan ini mempunyai keputusan yang lebih baik berbanding dengan yang lain. Keputusan yang diperolehi adalah setara dengan penemuan secara teori.

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I certify that a Thesis Examination Committee has met on 28 December 2015 to conduct the final examination of Lawan Sirajo Bichi on his thesis entitled "Modified Spline Functions and Chebyshev Polynomials for the Solution of Hypersingular Integrals Problems" in accordance with the Universities and University Colleges Act 1971 and the Constitution of the Universiti Putra Malaysia [P.U.(A) 106] 15 March 1998. The Committee recommends that the student be awarded the Doctor of Philosophy.

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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy.

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LIST OF ABBREVIATIONS

BCs	Boundary Conditions
HSI	Hypersingular integrals
CPV	Cauchy principal-value integrals
AQS	Automatic quadrature scheme
B	Closed region in d-dimensional Euclidean space
BS	B-Spline
D	Closed bounded connected set in R^2
K(x,y)	Regular or singular kernel
c_1, a_1 and b_1	Lower limits of integrals
c_2, a_2 and b_2	Upper limits of integrals
$S_\Lambda(P)$	Modified spline function of type $(0,2)$
QT	Quadrature type
GLQ	Gauss-Legendre quadrature
GJQ	Gauss Jacobi quadrature
GChQ	Gauss Chebyshev quadrature
GLgQ	Gauss Laguerre quadrature
GHQ	Gauss Hermite quadrature
$C^{N,\alpha}[-1,1]$.	Class of function which is N times continuous differentiable and belong to Hölder continuous functions
$C^{2,\gamma}(\Omega)$,	Class of function which is 2 times continuous partially differentiable and satify Hölder condition
CC	Clenshaw-Curtis Chebyshev quadrature methods
LP	Legendre Polynomial
ChP	Chebyshev Polynomials
QF	Quadrature formula
AS	Algebraic singularity
LS	Logarithmic singularity
CF	Cubature formula

CHAPTER 1

INTRODUCTION

1.1 Background

Splines can be considered as a mathematical model that associate a continuous representation of a curve or surface with a discrete set of points in a given space (Weston, 2002). The general form of cubic spline is given by

$$S(x) = \begin{cases} s_0(x), & \text{if } x_0 \leq x \leq x_1, \\ s_1(x), & \text{if } x_1 \leq x \leq x_2, \\ \vdots & \vdots \\ s_{n-1}(x), & \text{if } x_{n-1} \leq x \leq x_n, \end{cases} \tag{1.1}$$

where each $s_i(x)$ is cubic polynomial for n data points say $(x_0, y_0), (x_1, y_1), (x_2, y_2), \cdots (x_n, y_n)$.

A cubic spline interpolant S, for given function h satisfies

1. S is a cubic polynomial, $s_i(x)$ on $[x_i, x_{i+1}]$, for $i = 0, 1, \cdots, n-1$
2. $S(x_i) = h(x_i)$, for $i = 0, 1, 2, \cdots, n-1, n$
3. $S_{i+1}(x_{i+1}) = S_i(x_{i+1})$, for $i = 0, 1, 2, \cdots, n-2$
4. $S'_{i+1}(x_{i+1}) = S'_i(x_{i+1})$, for $i = 0, 1, 2, \cdots, n-2$
5. $S''_{i+1}(x_{i+1}) = S''_i(x_{i+1})$, for $i = 0, 1, 2, \cdots, n-2$
6. One of the following boundary conditions is satisfied
   - $S''(x_0) = S''(x_n) = 0$ (free or natural BCs)
   - $S'(x_0) = h'(x_0)$ and $S'(x_n) = h'(x_n)$ (clamped BCs)

The subject of singular integrals is highly significant tool in the pure Mathematics as well as the applied mathematics. Significant contribution had been made by many researchers in both singular and hypersingular integrals. The evaluation of HSI has been a case of interest to many researchers tackling many unsolved problems. To achieve this, there is the need to implement various techniques via approximate methods for evaluating HSI. In some cases, however, require the transformation of HSIs into singular or weakly singular integrals by using various techniques proposed in Clenshaw and Curtis (1960); Monegato (1960); Hasegawa and Torii (1991); Martin and Rizzo (1996); Eskhuvatov et al. (2011); Eskhuvatov and Nik Long (2011); Tadeu and Antonio (2012). Others, may require the numerical computation of finite part integrals by various quadrature or cubature formulas as in the research work done in Kutt (1975); Hui and Shia (1999); Colm and Rokhlin (2001); Yang (2012). Some ideas used the quadrature formula as in the work of Clenshaw and Curtis (1960); Hasegawa and Torii (1991); Eskhuvatov et al. (2011); Obayis et al. (2013), which take advantage of the collocation points to solve the Cauchy principalvalue and hypersingular integrals problems.

Consider the Hadamard finite-part integral (or hypersingular integral) of the form

$$H_p(a,b;s,h) = \oint_a^b \frac{h(t)}{(t-s)^{p+1}}, s \in (a,b), p = \{1,2\} \tag{1.2}$$

with $p+1$-order singularity and s is the singular point.

Definition 1.1.1 (Boykov et al. (2009) and Zhang et al. (2009)) HSI (1.2) must be understood in the Hadamard finite-part sense and is defined as

$$\oint_a^b \frac{h(t)}{(t-s)^{p+1}}dt = \lim_{\epsilon\to 0}\left\{\int_a^{s-\varepsilon} \frac{h(t)}{(t-s)^{p+1}}dt + \int_{s+\varepsilon}^{b} \frac{h(t)}{(t-s)^{p+1}}dt - \frac{2h^{(p-1)}(s)}{\varepsilon}\right\}, \tag{1.3}$$

$h(t)$ is said to be finite-part integrable (or integrable in the Hadamard sense) with the kernel $(t-s)^{-p-1}$ if the limit on the right-hand side of (1.3) exist.

An important and widely used definition of HSI in the society of engineers is that if $h(t)$, $a \le t \le b$, satisfies a Hölder continuous first-derivative condition

$$|h(t)-h(x)-(t-x)h'(x)| \le A|t-x|^{\alpha+1}, \tag{1.4}$$

where A is a positive constant and $\alpha \in (0,1]$.

The HSI is defined as

$$H(h,x) = \oint_{-1}^{1} \frac{h(t)}{(t-x)^2}dt = \lim_{\epsilon\to 0}\left[\left(\int_{-1}^{x-\epsilon} + \int_{x+\epsilon}^{1}\right)\frac{h(t)}{(t-x)^2}dt - \frac{2h(x)}{\epsilon}\right], \tag{1.5}$$

where this limits of integration exists and bounded. The high order accuracy was obtained by Hui and Shia (1999) for hypersingular integrals with second-order singularities of the form

$$H(h,x) = \oint_a^b \frac{w(t)h(t)}{(t-x)^2}dt, \tag{1.6}$$

in which the Gaussian quadrature rule have been used based on the Legendre and Chebyshev series expansion.

Differentiation of Cauchy principle-value integral (CPVI)

$$C(h,x) = \int_{-1}^{1} \frac{w(t)h(t)}{t-x} dt \tag{1.7}$$

with respect to the singular point x, gives

$$H(h,x) = \int_{-1}^{1} \frac{w(t)h(t)}{(t-x)^2} dt = \frac{d}{dx}\int_{-1}^{1} \frac{w(t)h(t)}{t-x} dt, \;\; x \in (-1,1) \tag{1.8}$$

which is also another definition of HSI according to Hui and Mukherjee (1997). Thus HSI represent a natural extension of singular integrals in the Cauchy principal-value (CPV). i.e

$$H(h,x) = \frac{d}{dx} C(h,x). \tag{1.9}$$

In order to approximate integration in two or more dimensions, Let B designate a closed region in d-dimensional Euclidean space and let dV designate the d-dimensional volume element in Davis and Rabinowitz (1984). Find fixed points $P_1, P_2, \cdots, P_n$ (preferably in B) and fixed weights $w_1, w_2, \cdots, w_n$ such that

$$\int_B w(P)h(P)dV \approx \sum_{k=1}^{n} w_k h(P_k). \tag{1.10}$$

This is a useful approximation to the integral on the left for a reasonably large class of functions of d variables defined on B.

The problem of approximating double integral of the form

$$H(h) = \int\int_D K(x,y)h(x,y)dA, \tag{1.11}$$

where $K(x,y)$ is a regular or singular kernel and D is closed bounded connected set in R^2 was studied by Eshkuvatov et al. (2013). In particular, the problem of evaluations of double integrals with the function of algebraic singularity

$$H(h) = \int_D h(\bar{x})|\bar{x} - \bar{x_0}|^{\gamma-2} dA, \; 0 < \gamma \leq 1, \tag{1.12}$$

where D is a closed bounded simple connected region in $\mathscr{R}^2$ and $\bar{x} = (x,y) \in D$ are variables and $\bar{x_0} = (x_0, y_0)$ is a fixed point in D was studied. Double integral in (1.12) has algebraic singularity at a point of the plane D where $|\bar{x} - \bar{x_0}| \to 0$.

Therefore the numerical calculation of (1.12) requires a care about subtle point. Various approximations of an integral

$$H(h) = \int_{\Omega} W(\mathbf{x})h(\mathbf{x})d\mathbf{x},$$

where $\Omega \in \Re^n$, and $W(\mathbf{x}) \geq 0$, $\forall \mathbf{x} \in \Re^n$, $n \geq 2$, by

$$H(h) = Q(h) + R(h),$$

where $Q(h)$ is the cubature formula (CF) and $R(h)$ is the remainder are presented by Cools and Rabinowitz (1993) and Cools (2003). To solve multivariate singular integrals problems there is need to find an efficient approximate formulas as in Stroud (1973); Davis and P. (1984); Evans (1993); Krommer and Ueberhuber (1998).

1.2 Problem statement

Many problems of multivariate integration problems arise in applications but the analytic solutions does not exist. Hence it become necessary to use the numerical techniques to arrive at the solutions. One such approaches to numerical solutions of double integrations problems is by using the spline interpolation. Although the modified spline function $S_{\Lambda}(P)$ of type $(0,2)$ was established theoretically to have interpolate the density functions in the double integration problems, the justifications in the accuracy has not been established numerically.

In the evaluation of HSIs problems, there the need to develop accurate AQSs via suitable approximations approach. Some researches have been conducted previously, for the constructions of AQSs particularly with the weight functions $w_0 = 1,\ w_1 = \sqrt{1-x^2}$ and $w_2 = \frac{1}{\sqrt{1-x^2}}$ for some HSIs problems. Additionally, error estimation was obtained for w_0 case only. Hence the need to investigate constructions of AQSs for similar and other weight functions via different approximations approaches and also obtain the error estimations for those weight functions that have not been considered. More investigations are needed for the exactness of the AQSs.

1.3 Objectives of the thesis

The problems of double integrals of the form

$$H_k(x,y) = \begin{cases} \iint\limits_{\Omega} \frac{h(x,y)}{|\bar{x}-\bar{x}_0|^{2-\gamma}} dA, 0 \leq \gamma \leq 1, & k = 1, \\ \iint\limits_{\Omega} h(x,y) \log|\bar{x}-\bar{x}_0^*| dA, & k = 2, \end{cases} \tag{1.13}$$

where $\Omega=[a_1,a_2]\times[b_1,b_2]$, $\bar{x}=(x,y)\in\Omega$ and fixed point $\bar{x}_0^*=(x_0^*,y_0^*)\in\Omega$, the density function $h(\bar{x})$ is assumed continuous and smooth enough on the rectangle Ω and belong to the class of function $C^{2,\gamma}(\Omega)$, i.e. $h(\bar{x})$, $h_x(\bar{x})$, $h_y(\bar{x})$, $h_{xx}(\bar{x})$, $h_{yy}(\bar{x})$ and $h_{xy}(\bar{x})=h_{yx}(\bar{x})$ in Ω are all continuous and all second partial derivatives satify Hölder condition are considered. The aims of the thesis here are:

- To construct cubature formulas and develop Maple codes for the constructed cubature formulas in the two cases $i\in\{1,2\}$ for double integrals with algebraic and logarithmic singularities respectively, on a rectangle Ω using the modified spline function $S_\Lambda(P)$ of type $(0,2)$.
- To obtain the exactness and provide numerical results of the cubature formulas for the two cases $i\in\{1,2\}$ together with tested examples each for linear and quadratic functions.

Furthermore, the problem of Hadamard type hypersingular integral (HSI) of the form

$$H_i(h,x)=\frac{w_i(x)}{\pi}\,=\!\!\!\!\!\!\int_{-1}^{1}\frac{h(t)}{w_i(t)(t-x)^2}dt,\, x\in(-1,1),\, i\in\{1,2,3,4\}, \tag{1.14}$$

where $w_1(t)=\sqrt{1-t^2}$, $w_2(t)=\dfrac{1}{\sqrt{1-t^2}}$, $w_3(t)=\sqrt{\dfrac{1-t}{1+t}}$ and $w_4(t)=\sqrt{\dfrac{1+t}{1-t}}$ are the weights and $h(t)$ is a smooth function are considered. The aims of the thesis here are:

- To construct an automatic quadrature schemes (AQSs) together with their Maple codes and obtain error estimations in each case for $i\in\{1,2,3,4\}$ via approximating the density function $h(t)$ by the first, second, third and fourth kind truncated series of Chebyshev polynomials, respectively.
- To obtain exactness for the degree 3 polynomial functions and obtain numerical results of the AQSs each for $i\in\{1,2,3,4\}$ for the tested density function $h(t)$ as polynomial and rational functions. However, compare the efficiency and accuracy of the AQSs constructed with other known methods in the available literature.

1.4 Scope of the study

The research work was based on the following scopes;

- The solution of double integration problems in the rectangular domain using the modified spline function $S_\Lambda(P)$ of type $(0,2)$.
- Use of Gauss chebyshev quadrature formula approaches to solve the hypersingular integrations problems by approximating the density functions with first, second, third and fourth kind truncated series of chebyshev polynomials.

- Use of Maple 14 to develop the codes in both cubature formulas and automatic quadrature formulas to solve the double and hypersingular integrations problems.

1.5 Limitations of the study

Our investigation in this research work is limited the use of test function as linear and quadratic function on the constructed cubature formulas (3.14) with $k \in \{1,2\}$ for double integration with algebraic and logarithmic singularities, $H_k(x,y)$ for $k=2$ in (3.1). In an attempt to test the methods with the rational function due to the large computations involved in the method and the number of iterations needed to arrive at the solutions, it was found impossible to manage this with smaller processing unit computers. A powerful and higher processing computing machine (HPC) which understand the Maple computing is needed to handle the job.

1.6 Outline of the thesis

In Chapter 1, motivation and reason of the research is given. Problem statement, objectives, scope of the study, limitations, outline of the thesis and basic concepts and definitions related to research work are discussed.

Chapter 2 is devoted to earlier research on cubature and quadrature in numerical integration as well as their approach to the double integration and hypersingular integration problems, respectively.

Chapter 3 presents the concept of double integration by spline polynomial. Demonstrated the construction of cubature formulas for double integration problems with algebraic and logarithmic singularities. Exactness of the obtained cubature formulas each for linear and quadratic functions and finally numerical results and discussion are provided and discussed.

Chapter 4 provides the mathematical concepts of the first and second kind Chebyshev polynomials and hypersingular integrals. The detail construction of automatic quadrature schemes for bounded and unbounded hypersingular integrals and rate of convergence of the suggested methods are discussed. Additionally, the exactness of the AQSs constructed each for polynomials of degree 3 are Shown and finally numerical results are given and discussed.

Chapter 5 provides the mathematical concepts of the third and fourth kind Chebyshev polynomials and hypersingular integrals. The construction of automatic quadrature schemes for semi bounded solutions of hypersingular integrals and the rate of convergence of the suggested methods are presented. Additionally, the exactness of the AQSs each for polynomials of degree 3 are shown and finally numerical results are given and discussed.

Finally, Chapter 6 gives conclusion of the research work. Some future works are also suggested on Cubature and Quadrature formulas.

1.7 Basic concepts and definitions

To facilitate understanding in this thesis write up, the following concepts and definitions are useful. Beginning with the continuous orthogonality which can be seen from the following

Definition 1.7.1 (Mason and Handscomb (2003)) *Two functions $h_1(t)$ and $h_2(t)$ in $L_2[c_1, c_2]$ are said to be orthogonal on the interval $[c_1, c_2]$ with respect to weight function $w(t)$ if*

$$\langle h_1, h_2 \rangle = \int_{c_1}^{c_2} w(t) h_1(t) h_2(t) dt = 0. \tag{1.15}$$

Infact, it is possible to convert continuous orthogonality relationship (1.15) into a discrete orthogonality relationship by replacing the integral with a summation and the result here is in general, only approximately true. Particularly, in case of discrete orthogonality for trigonometric functions or Chebyshev polynomials, there are many cases which the formulas have been shown to hold exactly by Mason and Handscomb (2003).

1.7.1 Standard Quadrature Formula of Gauss-type

A quadrature rule is an approximation of the definite integral of a function, usually stated as a weighted sum of function values at specified points within the domain of integration (Teubner and Leipzig, 1993). An n-point Gaussian quadrature rule, named after Carl Friedrich Gauss, is a quadrature rule constructed to yield an exact result for polynomials of degree $2n-1$ or less by a suitable choice of the points x_i and weights w_i for $i = 1, \cdots, n$. The domain of integration for such a rule is conventionally taken as $[-1, 1]$, so the rule is stated as

$$\int_{-1}^{1} h(x) dx \approx \sum_{i=1}^{n} w_i h(x_i). \tag{1.16}$$

Gaussian quadrature as above will only produce accurate results if the function $h(x)$ is well approximated by a polynomial function within the range [-1, 1]. The method is not, for example, suitable for functions with singularities. However, if the integrated function can be written as $h(x) = \omega(x) g(x)$, where $g(x)$ is approximately polynomial and $\omega(x)$ is known weight function, then alternative weights $w_i^{'}$ and points $x_i^{'}$ that depend on the weighting function $\omega(x)$ may give better results, where

$$\int_{-1}^{1} h(x)dx = \int_{-1}^{1} \omega(x)g(x)dx \approx \sum_{i=1}^{n} w_i^{'} h(x_i^{'}). \tag{1.17}$$

Common weighting functions include $\omega(x) = 1/\sqrt{1-x^2}$ (Gauss Chebyshev) and $\omega(x) = e^{-x^2}$ (Gauss Hermite).

1.7.2 Change of interval

If integral over $[c_1, c_2]$ need to be changed into an integral over $[-1, 1]$ then this change of interval can be done in the following way:

$$\int_{c_1}^{c_2} w(x)h(x)dx = \frac{c_2 - c_1}{2} \int_{-1}^{1} w_1(z)h(\frac{c_2 - c_1}{2}z + \frac{c_2 + c_1}{2})dz \tag{1.18}$$

$$\approx \sum_{i=1}^{n} w_i h(\frac{c_2 - c_1}{2}z_i + \frac{c_2 + c_1}{2}). \tag{1.19}$$

1.7.3 Gaussian rules

Let $\upsilon_n(x)$ denote a sequence of polynomials, where $\upsilon_n(x) \in \mathscr{P}$ and the polynomials $\upsilon_n(x)$ are orthogonal with respect to a weight function $w(x)$ over the interval $[c_1, c_2]$. We can write $\upsilon_n(x) = b_n p_n(x) + b_{n-1}p_{n-1}(x) + \cdots + b_0$, where $b_n \neq 0$ is the coefficient of x^n in $\upsilon_n(x)$, and $p_n(x)$ is an orthogonal polynomial. Then

$$\int_{c_1}^{c_2} w(x)\upsilon_i(x)\upsilon_j(x)dx = 0, \text{ for } i \neq j. \tag{1.20}$$

with the *Chrstoffel-Darbourx identity*

$$\sum_{k=0}^{n} \frac{\upsilon_k(x)\upsilon_k(y)}{\gamma_k} = \frac{\upsilon_{n+1}(x)\upsilon_n(y) - \upsilon_n(x)\upsilon_{n+1}(y)}{\alpha_n \gamma_n (x-y)}, \tag{1.21}$$

where

$$\alpha_n = \frac{b_{k+1}}{b_k}, \;\; \gamma_n = \int_{c_1}^{c_2} w(x)\upsilon_k^2(x)dx. \tag{1.22}$$

Now, let $y = x_i$, where x_i are the zeros of $\upsilon_n(x)$, then

$$\sum_{k=0}^{n-1} \frac{\upsilon_k(x)\upsilon_k(x_i)}{\gamma_k} = \frac{\upsilon_{n+1}(x)\upsilon_n(x_i) - \upsilon_n(x)\upsilon_{n+1}(x_i)}{\alpha_n \gamma_n (x - x_i)}. \tag{1.23}$$

Multiply both sides of (1.23) by $w(x)\upsilon_0(x)$ and integrate over $[c_1,\ c_2]$, then applying (1.20) we have

$$\upsilon_0(x_i) = -\frac{\upsilon_{n+1}(x_i)}{\alpha_n \gamma_n} \int_{c_1}^{c_2} w(x) \frac{\upsilon_0(x)\upsilon_n(x)}{x - x_i} dx. \tag{1.24}$$

Recalling the definition of the Lagrangian interpolation polynomial

$$l_i(x) = \frac{\pi_n(x)}{(x - x_i)\pi_n'(x_i)} = \frac{\upsilon_n(x)}{(x - x_i)\upsilon_n'(x_i)}, \tag{1.25}$$

and since for some constant $\upsilon_0(x) = c$, we find from (1.24) and (1.25) that

$$\begin{aligned} 1 &= -\frac{\upsilon_{n+1}(x_i)}{\alpha_n \gamma_n} \int_{c_1}^{c_2} w(x) \frac{\upsilon_n(x)}{x - x_i} dx \\ &= -\frac{\upsilon_{n+1}(x_i)\upsilon_n'(x_i)}{\alpha_n \gamma_n} \int_{c_1}^{c_2} w(x) l_i(x) dx \\ &= -\frac{\upsilon_{n+1}(x_i)\upsilon_n'(x_i)}{\alpha_n \gamma_n} w_i \end{aligned} \tag{1.26}$$

where

$$w_i = -\frac{b_{n+1}\gamma_n}{b_n \upsilon_{n+1}(x_i)\upsilon'(x_i)} \text{ for } i = 1, \cdots, n. \tag{1.27}$$

The error is given by

$$E_n = \frac{\gamma_n}{b_n^2 (2n)!} h^{(2n)}(\xi),\ c_1 < \xi < c_2. \tag{1.28}$$

Note that for the Legendre polynomials $P_n(x)$ these formulae give

$$\begin{aligned}
\gamma_n &= \int_{-1}^{1} P_n^2(x)dx = \frac{2}{2n+1}, \\
b_n &= \frac{(2n)!}{2^n(n!)^2}, \\
w_i &= -\frac{2}{(n+1)P_{n+1}(x_i)P_n'(x_i)}, && (1.29) \\
E_n &= \frac{2^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} h^{(2n)}(\xi). && (1.30)
\end{aligned}$$

Consider quadrature rules of the form

$$I_{c_1}^{c_2}(h) = \int_{c_1}^{c_2} h(x)dx = \sum_{i=0}^{m} w_i h(x_i), \tag{1.31}$$

where x_i are not equally spaced. Replacing h by an interpolating polynomial $p_n(x)$ constructed at the points x_i, $i = 0, 1, \cdots, n$, then the polynomial will have Lagrangian form

$$p_n(x) = l_0(x)h(x_0) + \cdots + l_n(x)h(x_n), \tag{1.32}$$

where $l_i(x)$, $i = 0, 1, \cdots, n$, are defined by

$$l_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}. \tag{1.33}$$

By integrating (1.32) over $c_1 \leq x \leq c_2$, we get the right hand side of (1.31), in which case the weights w_i are given by

$$w_i = \int_{c_1}^{c_2} l_i(x)dx, \ 0 \leq i \leq n, \tag{1.34}$$

For an equally-spaced nodes x_i this procedure leads to a different method of deriving the Newtons-cotes quadrature formulas. The error term

$$E(x) = (x - x_0)(x - x_1)\cdots(x - x_n)\frac{h^{n+1}(\xi)}{(n+1)!}, \ c_1 < \xi < c_2 \tag{1.35}$$

$h^{n+1}(\xi)$ is continuous and ξ depends on x on integration over the interval $[c_1, c_2]$ gives

$$I_{c_1}^{c_2}h - \sum_{i=0}^{n} w_i h(x_i) = \frac{1}{(n+1)!}\int_{c_1}^{c_2} \pi_{n+1}(x)h^{n+1}(\xi), \tag{1.36}$$

where $\pi_{n+1}(x) = (x-x_0)(x-x_1)\cdots(x-x_n)$. Thus, the quadrature rule (1.31) is exact if $h \in \mathscr{P}_n$ because since $h^{n+1}(x) \equiv 0$ the right side of (1.36) vanishes. The rule (1.31) is exact for any linear combination of functions h and g if it is exact for the functions h and g separately. Thus, if α and β are any arbitrary real numbers, we have

$$\int_{c_1}^{c_2}(\alpha h(x)+\beta g(x))dx = I_{c_1}^{c_2}h + I_{c_1}^{c_2}g = \sum_{i=0}^{n} w_i[\alpha h(x_i)+\beta g(x_i)]. \tag{1.37}$$

This shows that the rule (1.31) is exact for $h \in \mathscr{P}_n$ if it is exact for the monomials $1, x, x^2, \cdots, x^n$. In fact, the rule (1.31) is exact for x^j if

$$\int_{c_1}^{c_2} x^j dx = \sum_{i=0}^{n} w_i x_i^j. \tag{1.38}$$

Since the left side of (1.38) is known, we take $j = 0, 1, \cdots, 2n+1$ and obtain a system $(2n+2)$ equations to solve $2n+2$ unknowns w_i and for $i = 0, 1, \cdots, n$. If this system has a solution, the resulting quadrature rule will be exact for $h \in \mathscr{P}_n$ for $j, k < n$, so that

$$\sum_{i=0}^{n} w_i p_j(x_i) p_k(x_i) = \int_{c_1}^{c_2} w(x) p_j(x) p_k(x) dx = \delta_{jk}. \tag{1.39}$$

Thus

$$\langle h, g\rangle = \sum_{i=0}^{n} w_i h(x_i) g(x_i). \tag{1.40}$$

We will develop the error (1.36) in terms of the divided differences. Since

$$h(x) - p_n(x) = \pi_{n+1}(x) h[x, x_0, \cdots, x_n], \tag{1.41}$$

we have

$$I_{c_1}^{c_2}h - \sum_{i=0}^{n} w_i h(x_i) = \int_{c_1}^{c_2} \pi_{n+1}(x) h[x, x_0, \cdots, x_n] dx. \tag{1.42}$$

If $h[x,x_0,\cdots,x_n] \in \mathscr{P}_m,\ m>0$, then $h[x,x_0,\cdots,x_{k+1}] \in \mathscr{P}_{m-1}$. This result follows from

$$h[x,x_0,\cdots,x_n] = \frac{h[x_0,\cdots,x_n]-h[x,x_0,\cdots,x_{n-1}]}{x_n-x_0}, \tag{1.43}$$

called a divided difference, which gives

$$h[x,x_0,\cdots,x_{k+1}] = \frac{h[x_0,\cdots,x_{k+1}]-h[x,x_0,\cdots,x_k]}{x_{k+1}-x}, \tag{1.44}$$

and since the numerator on the right side is a polynomial of degree m and has $(x-x_{k+1})$ as one of the factors, then $h \in \mathscr{P}_{m-1}$. Hence, if $h \in \mathscr{P}_{2n+1}$, we can show by induction that $h[x,x_0,\cdots,x_n] \in \mathscr{P}_n$. Now, let $\{p_0,p_1,\cdots,p_{n+1}\}$ be a set of orthogonal polynomials $[c_1,\ c_2]$, and let $p_r \in \mathscr{P}_r,\ r=0,1,\cdots,n+1$. Then for some set of real numbers $\alpha_0,\alpha_1,\cdots,\alpha_n$, we have $h[x,x_0,\cdots,x_n] = \alpha_0 p_0+\alpha_1 p_1+\cdots+\alpha_n p_n$. Then, because of the orthogonality relations

$$\int_{c_1}^{c_2} p_r(x)p_s(x)dx \begin{cases} 0, & \text{for } r \neq s, \\ ||p_s||^2, & \text{for } r=s, \end{cases} \tag{1.45}$$

the right side of (1.42) is zero if $\pi_{n+1}(x)=\alpha p_{n+1}(x)$ for some real $\alpha \neq 0$.

The Gaussian quadrature rules cannot in general be used for functions that are defined only at discrete points since such rules require that the functions be evaluated at specific points ξ_t which are the zeros of the related polynomials. However, in some experimental cases where there is complete freedom of choosing the data of functional values at the specific nodes ξ, the corresponding Gaussian rules can be used to evaluate $I_{c_1}^{c_2}(h)$. The error bounds are virtually impossible to obtain in such cases. But if the data is mostly error free, then a very high order interpolating polynomial may be effectively used to obtain a significantly accurate result. There is no practical advantage in using a Gaussian quadrature if the data is noisy and some smoothing is needed prior to the application of a specific Gaussian quadrature rule.

It must also be noted that the Gaussian rules of all orders are also Riemann sums. These rules integrate exactly polynomials of any degree by a formula of the form (1.31).

1.7.4 Extended Gaussian Rules

The extended (repeated or compund) Gaussian rules are similar to the repeated trapezoidal, midpoint and Simpson's rules.

Theorem 1.7.1 (Abramowitz and Stegun (1972)) *If $p_{2n+1}(y) \in \mathscr{P}_{2n+1}$, then* *the formula*

$$\int_{c_1}^{c_2} w(x)p_{2n+1}(y)dy = \sum_{j=0}^{m} \gamma_i p_{2n+1}(y_i)$$

is exact if the points y_j, $j = 0,1,\cdots,m$, *are the zeros of the orthogonal polynomial* υ_{m+1}, *and* γ_j *are defined by*

$$\gamma_j = \int_{c_1}^{c_2} w(x) l_j(x) dx$$

Theorem 1.7.2 (Johnson and Riess (1977)) *Gaussian quadrature formula has precision* $2m+1$ *only if the points* x_j, $j = 0,1,\cdots,m$, *are the zeros of* υ_{m+1}.

Theorem 1.7.3 (Abramowitz and Stegun (1972)) *Let* $h(y) \in C^{2m+2}[c_1, c_2]$, *then the error in the Gaussian quadrature is*

$$I_{c_1}^{c_2} - I_m = \frac{h^{2m+2}(\xi)}{(2m+2)!} \int_{c_1}^{c_2} w(y) T_{m+1}^2(y) dy$$

where T_m *is the Chebyshev polynomial of the first kind.*

1.7.4.1 Gauss-Jacobi Rule

The Jacobi polynomials $P^{(\gamma,\sigma)}$ are the orthogonal with weight function $w(y) = (1-y)^{\gamma}(1+y)^{\sigma}$, $\gamma > -1$, $\sigma > -1$. The Gauss-Jacobi rule (also known as the Mehler quadrature formula) is defined by

$$\int_{-1}^{1} (1-y)^{\gamma}(1+y)^{\sigma} h(y) dy = \sum_{j=1}^{m} w_j h(y_j) + E, \tag{1.46}$$

where

$$w_j = -\frac{2m+\gamma+\sigma+2}{2m+\gamma+\sigma+1} \frac{\Gamma(m+\sigma+1)\Gamma(m+\gamma+\sigma+1)}{(m+1)!\Gamma(m+\gamma+\sigma+1)} \times \frac{2^{\gamma+\sigma}}{P_m^{\prime(\gamma+\sigma)}(y) P_{m+1}^{(\gamma+\sigma)}(y)}. \tag{1.47}$$

and the series form of Jacobi polynomials $P^{(\gamma,\sigma)}$ (Prem and Michael, 2005) is

$$P^{(\gamma,\sigma)}(y) = \frac{1}{2^m} \sum_{k=0}^{[m/2]} \binom{m+\gamma}{k} \binom{m+\sigma}{m-k} (y-1)^{m-k}(y+1)^k, \tag{1.48}$$

and the error term E_m in the m-point rule is

$$E_m = \frac{\Gamma(m+\gamma+1)\Gamma(m+\sigma+1)\Gamma(m+\gamma+\sigma+1)}{(2m+\gamma+\sigma+1)[\Gamma(2m+\gamma+\sigma+1)]^2} \times \frac{m!2^{2m+\gamma+\sigma+1}}{(2m)!} h^{2m}(\xi),\ \xi \in (-1,1). \tag{1.49}$$

The Gauss-Legendre rule is a special case of formula (1.47) with $\gamma = \sigma = 0$. The Gauss-Chebyshev rule is another special case with $\gamma = \sigma = -\frac{1}{2}$ For integrands with the Jacobi weight function $w(y) = (1-y)^{\gamma}(1+y)^{\sigma}$ in (Piessens and Branders, 1973) use the formulas

$$\int_{-1}^{1} (1-y)^{\gamma}(1+y)^{\sigma} g(y) \approx \sum_{k=0}^{M} b_k G_k(\gamma,\sigma) + E'_M, \tag{1.50}$$

$$\int_{-1}^{1} (1-y)^{\gamma}(1+y)^{\sigma} \ln\frac{1+y}{2} g(y)dy \approx \sum_{k=0}^{M} b_k I_k(\gamma,\sigma) + E_M^2, \tag{1.51}$$

where $g(y)$ is assume to have a rapidly convergent Chebyshev series expansion

$$g(y) = \sum_{k=0}^{\infty}{}' a_k T_k(y), \tag{1.52}$$

and

$$b_k = \frac{2}{M} \sum_{k=0}^{\infty}{}'' g(y_i) T_k(y_i),\ y_i = \cos\frac{i\pi}{M}, \tag{1.53}$$

$$G_m(\gamma,\sigma) = 2^{\gamma+\sigma+1} \frac{\Gamma(\gamma+1)\Gamma(\sigma+1)}{\Gamma(\gamma+\sigma+2)} 3F \left[\begin{matrix} m,-m,\gamma+1 \\ \frac{1}{2},\gamma+\sigma+2 \end{matrix} ;1 \right], \tag{1.54}$$

$$E_k^1 \approx a_{k+1}(G_{k+1}(\gamma,\sigma) - I_{k-1}(\gamma,\sigma)), \tag{1.55}$$

$$E_k^2 \approx a_{k+1}(I_{k+1}(\gamma,\sigma) - I_{k-1}(\gamma,\sigma)), \tag{1.56}$$

and $I_m(\gamma,\sigma)$ are obtained from the recurrence relation

$$(\gamma+\sigma+m+2)I_{m+1}(\gamma,\sigma) + 2(\gamma-\sigma)I_m(\gamma,\sigma) + (\gamma+\sigma-m+2)I_{m-1}(\gamma,\sigma) = 2G_m(\gamma,\sigma) - G_{m-1}(\gamma,\sigma) - G_{m+1}(\gamma,\sigma). \tag{1.57}$$

1.7.4.2 Gauss-Legendre Rule

This rule is a special case of the Gauss-Jacobi formula (1.47) with $\gamma = \sigma = 0$. The weight function $w(y) = 1$ and the orthogonal polynomials $\upsilon_j(y)$ are the Legendre polynomials $P_j(y),\ j = 0,\cdots$, with $p_j(1) = 1$. This rule on the interval $[-1,1]$ is given by (1.31), where the nodes y_j are the $j-th$ zero of P_m; the weight are given by

$$w_j = \frac{2}{(1-y_j^2)[P_m'(y_j)]^2}; \tag{1.58}$$

and the remainder is

$$R_m = \frac{2^{2m+1}(m!)^4}{(2m+1)[(2m)!]^3} h^{2m}(\xi), -1 < \xi < 1. \tag{1.59}$$

The Gauss-Legendre rule fore arbitrary interval $[c_1, c_2]$ is

$$\int_{c_1}^{c_2} h(y)dy = \frac{c_2-c_1}{2} \sum_{j=1}^{m} w_j h(y_j) + R_m \tag{1.60}$$

where the nodes are

$$y_i = \left(\frac{c_2-c_1}{2} x_j + \frac{c_2+c_1}{2}\right); \tag{1.61}$$

the related nodes x_j and the weights w_i are defined above; and

$$R_m = \frac{(c_2-c_1)^{2m+1} 2^{2m+1}(m!)^4}{(2m+1)[(2m)!]^3} h^{2m}(\xi),\ c_1 < \xi < c_2. \tag{1.62}$$

The rule (1.31) are exact for $h \in \mathscr{P}_{2m+1}$.

Using the first legendre polynomial

$$P_0(y) = 1, P_1(y) = y,\ P_2(y) = (3y^2-1)/2,\ P_3(y) = (2y^3-3y)/2,$$

we get:

1. For $m = 2$ in (1.31) we have the Gauss-Legendre rule with one node at $y = 0$ which is the zero of $P_1(y) : I_{-1}^{1} h = 2h(0)$, which is exact for $h \in \mathscr{P}_1$. This is comparable to the midpoint rule.
2. For $m = 1$ in (1.31) we have the Gauss-Legendre rule with two nodes at $y = \pm 1/\sqrt{3}$ which are the zeros of $P_2(y) : I_{-1}^{1} h = h(-1/\sqrt{3}) + h(1/\sqrt{3})$, which is exact for $h \in \mathscr{P}_3$. This is comparable to the Simpson's rule.
3. For $m = 2$ in (1.31) we have the Gauss-Legendre rule with three nodes at $y = 0, \pm\sqrt{3/5}$ which is the zero of $P_3(y) : I_{-1}^{1} h = 2[5h(-\sqrt{3/5}) + 8h(0) + 5h(0) + 5h(\sqrt{3/5})]/9$, which is exact for $h \in \mathscr{P}_5$.

For the Gauss-Legendre rule, an interval $[c_1, c_2]$ can be transformed into $[-1, 1]$ by using the transformation

$$c_1 = \frac{c_2+c_1}{2} + \frac{c_2-c_1}{2}\xi,\ \xi \in [-1, 1]. \tag{1.63}$$

Then the Gauss-Legendre quadrature rule becomes

$$Hh = \frac{c_2 - c_1}{2} \sum_{k=1}^{m} w_k h(\xi_k). \tag{1.64}$$

where the nodes ξ_k are the m zeros of the $n-th$ degree Legendre polynomials.

1.7.4.3 Gauss-Laguerre Rule.

A Gaussian quadrature over the interval $[0,\infty)$ with weight function $w(x) = e^{-x}$ (Davis and Rabinowitz, 1984) is Gauss-Laguerre. The abscissae for quadrature order n are given by the roots of the Laguerre polynomials $L_n(x)$. The weights are

$$w_i = -\frac{A_{n+1}\gamma_n}{A_n L'_n(x_i) L_{n+1}(x_i)} = \frac{A_n}{A_{n-1}} \frac{\gamma_{n-1}}{L_{n-1}(x_i) L'_n(x_i)}, \tag{1.65}$$

where A_n is the coefficient of x^n in $L_n(x)$, given by $A_n = \frac{(-1)^n}{n!}$. Thus, $\frac{A_{n+1}}{A_n} = -\frac{1}{n+1}$, and $\frac{A_n}{A_{n-1}} = -\frac{1}{n}$. Also, $\gamma_n = \int_0^\infty w(x)[L_n(x)]^2 dx = 1$, which gives

$$\begin{aligned} w_i &= \frac{1}{(n+1)L'_n(x_i)L_{n+1}(x_i)} = \frac{1}{nL_{n-1}(x_i)L'_n(x_i)}, \\ &= \frac{1}{x_i[L'_n(x_i)]^2} = \frac{x_i}{(n+1)^2[L_{n+1}(x_i)]^2} \end{aligned} \tag{1.66}$$

The error term is given by

$$E_n = \frac{(n!)^2}{(2n)!} h^{(2n)(\xi)}. \tag{1.67}$$

1.7.4.4 Gauss-Hermite Rule.

This is a Gauss quadrature over the interval $(-\infty,\infty)$ with weight function $w(x) = e^{x^2}$ (Davis and Rabinowitz, 1984). The nodes for quadrature of order n are given by the roots x_i of the Hermite polynomials H_n, which occur symmetrically about 0. Th weights are

$$w_i = -\frac{A_{n+1}\gamma_n}{A_n H'_n(x_i) H_{n+1}(x_i)} = \frac{A_n}{A_{n-1}} \frac{\gamma_{n-1}}{H_{n-1}(x_i) H'_n(x_i)}, \tag{1.68}$$

where A_n is the coefficient of x^n in $H_n(x)$. For Hermite polynomials, $A_n = 2^n$, so $\frac{A_{n+1}}{A_n} = 2$. Additionally, $\gamma_n = \sqrt{\pi} 2^n n!$, so (see Abramowitz and Stegun 1968, p.

890).

$$w_i = -\frac{2^{n+1} n! \sqrt{\pi}}{H_{n+1}(x_i) H_n'(x_i)} = \frac{2^n (n-1)! \sqrt{\pi}}{H_{n-1}(x_i) H_n'(x_i)}$$
$$= \frac{2^{n+1} n! \sqrt{\pi}}{\left[H_n'(x_i)\right]^2} = \frac{2^{n+1} n! \sqrt{\pi}}{\left[H_{n+1}(x_i)\right]^2} = \frac{2^{n-1} n! \sqrt{\pi}}{n^2 [H_{n-1}(x_i)]^2}, \tag{1.69}$$

where the following recurrence relations is used:

$$H_n'(x) = 2nH_{n-1} = 2xH_n(x) - H_{n+1}(x).$$

The error term is

$$E_n = \frac{n! \sqrt{\pi}}{2^n (2n)!} h^{(2n)(\xi)}. \tag{1.70}$$

The nodes and weights can be computed analytically for small n as:

$$n = 2: \quad x_i = \pm\sqrt{2}, \quad w_i = \frac{1}{2}\sqrt{\pi}, \; i \in \{1,2\}$$
$$n = 3: \quad x_0 = 0, \quad w_i = \frac{2}{3}\sqrt{\pi},$$
$$x_i = \pm\frac{1}{2}\sqrt{6}, \quad w_i = \frac{\sqrt{\pi}}{6}, \; i \in \{1,2\}$$
$$n = 4: \quad x_i = \pm\sqrt{\frac{3-\sqrt{6}}{2}}, \quad w_i = \frac{\sqrt{\pi}}{4(3-\sqrt{6})}, \; i \in \{1,2\}$$
$$x_i = \pm\sqrt{\frac{3+\sqrt{6}}{2}}, \quad w_i = \frac{\sqrt{\pi}}{4(3+\sqrt{6})}, \; i \in \{3,4\}.$$

1.7.4.5 Gauss-Radau Rule.

A Gaussian quadrature-like formula for numerical estimation of integrals. It requires $m+1$ points and fits all polynomials to degree $2m$, so it effectively fits exactly all polynomials of degree $2m-1$. It uses a weight function $w(x) = 1$ in which the endpoint -1 in the interval $[-1,1]$ is included in a total of n abscissae, $r - n - 1$ free abscissae. The general formula is

$$\int_{-1}^{1} h(x)dx = \frac{2}{n^2} h(-1) + \sum_{i=2}^{n} w_i h(x_i). \tag{1.71}$$

The free nodes for $i=2,\cdots,n$ are the roots of the polynomial $\frac{P_{n-1}(x)+P_n(x)}{1+x}$, where $P_n(x)$ is a Legendre polynomial. The weights of the free nodes are

$$w_i = \frac{1-x_i}{n^2[P_{n-1}(x_i)]^2} = \frac{1}{(1-x_i)\left[P'_{n-1}(x_i)\right]^2},\ i=1,\cdots,n. \tag{1.72}$$

The error term is

$$E_n = \frac{2^{2n-1}n[(n-1)!]^4}{[(2n-1)!]^3}h^{(2n-1)}(\xi),\ -1<\xi<1. \tag{1.73}$$

1.7.4.6 Gauss-Lobatto Rule.

Also known as Lobatto quadrature (Abramowitz and Stegun, 1972), named after Dutch mathematician Rehuel Lobatto. It is similar to Gaussian quadrature with the following differences:

1. The integration points include the end points of the integration interval.
2. It is accurate for polynomials up to degree $2n-3$, where n is the number of integration points (Quarteroni et al., 2000) .

Lobatto quadrature of function $h(x)$ on interval $[-1,\ 1]$: When the Gaussian formula (1.31) is used with the polynomials $P'_{n-1}(x)$, where $P_n(x)$ are the Legendre polynomials, we get Lobatto's rule:

$$\int_{-1}^{1} h(x)dx = \frac{2}{n(n-1)}[h(1)+h(-1)] + \sum_{i=1}^{n-1} w_i h(x_i) + R_n, \tag{1.74}$$

where the quadrature points x_i is the $(i-1)-st$ zero of $P'_{n-1}(x)$; this formula is exact if $h \in \mathscr{P}_{2n-1}$, and the weights $w_i = \frac{2}{n(n-1)[P_{n-1}(x_i)]^2}$ for $x_i \neq 1$; and

$$R_n = \frac{-n(n-1)^3 2^{2n-1}[(2n-1)!]^4}{(2n-1)[(2n-2)!]^3}h^{2n-2}(\xi),\ -1<\xi<1. \tag{1.75}$$

The 3−point Lobbato rule is Simpson's rule.

1.7.4.7 Gauss-Chebyshev Rule.

In the quadrature rule

$$\int_{c_1}^{c_2} w(x)h(x)dx = \sum_{i=0}^{n} w_i h(x_i), \tag{1.76}$$

the weight w_i and the nodes x_i can be found for different orthogonal polynomials approximations of $h(x)$ such that formula (1.76) is exact for all $h \in \mathscr{P}_{2n+1}$.

Thus, in particular, if $[c_1, c_2]$ is taken as $[-1, 1]$ and $w(x) = (1-x^2)^{-1/2}$, the orthogonal polynomial are the Chebyshev polynomials $T_N(x)$ of the first kind, and the resulting formulas are known as the Gauss-Chebyshev rule. Thus, by taking the interpolating polynomials as

$$p_n(x) = \sum_{i=0}^{n} l_i(x) h(x_i), \tag{1.77}$$

where x_i are the zeros of $T_n(x)$. Then, in view of (1.47) the weights w_i are given by

$$w_i = -\frac{\pi}{T_{n+1}(x_i) T_n'(x_i)}. \tag{1.78}$$

Putting $x = \cos\theta$, we have $T_n(x) = \cos n\theta$, and $T_n'(x) = \frac{n \sin n\theta}{\sin\theta}$. Now we write $x_i = \cos\theta_i$. Then

$$\begin{aligned} T_{n+1}(x_i) &= \cos(n+1)\theta_i = \cos n\theta_i \cos\theta_i - \sin n\theta_i \sin\theta \\ &= \mp\sqrt{1-x_i}, \end{aligned}$$

since $\cos n\theta = 0$,

$$T_n'(x_i) = \frac{n \sin n\theta_i}{\sin\theta_i} = \frac{\pm n}{\sqrt{1-x_i^2}},$$

which gives

$$w_i = \frac{\pi}{n} \tag{1.79}$$

This shows that for all Chebyshev rules the weights are all equal. The error in the $n-$point rule is given by

$$E_n = \frac{2\pi}{2^{2n}(2n)!} h^{(2n)}(\xi), \; -1 < \xi < 1. \tag{1.80}$$

If we choose $[c_1, c_2] = [-1, 1]$, $w(x) = (1-x^2)^{-1/2}$, and the polynomials $q_i(x)$ as the normalized Chebyshev polynomials

$$q_i(x) = \begin{cases} \sqrt{\frac{2}{\pi}} T_i(x) & \text{for } i = 1, 2, \cdots, n-1 \\ \sqrt{\frac{1}{\pi}} T_0(x) & \text{for } i = 0. \end{cases}$$

The nodes ξ_i for the $n-$point quadrature are zero of $T_n(x)$, defined by

$$\xi_i = \cos\frac{(2i-1)\pi}{2n}, \; i = 1, 2, \cdots, n. \tag{1.81}$$

The rule with ξ_i given by (1.82) and the weight (1.78) is of degree $2n-1$, and is known as the *open Gauss-Chebyshev rule*, since the endpoints are not included as the nodes. The word 'open' is generally omitted since all Gaussian rules with positive weight function are of the open type. This rule is also known as Fejér's first integration formula

$$\int_{-1}^{1} h(x)dx = \sum_{i=1}^{n} w_i h\left(\cos\frac{(2i-1)\pi}{2n}\right),\ h \in \mathscr{P}_{n-1} \tag{1.82}$$

where the weights w_i are given by

$$w_i = \frac{2}{\pi}\left[1-2\sum_{k=1}^{[n/2]}\frac{\cos(2k\theta_k)}{4k^2-1}\right]. \tag{1.83}$$

The (open) Gauss-Chebyshev rule is related to the midpoint rule with $w(x)=1$, which is defined by

$$H_{c_1}^{c_2}h \approx h\sum_{i=1}^{n} h\left(c_1+\frac{(2i-1)h}{2}\right),\ h=\frac{c_2-c_1}{2}. \tag{1.84}$$

This is easily seen by setting $[c_1,c_2]=[0,\pi]$ and $x=\cos\theta$; then the above midpoint rule changes to

$$\int_{-1}^{1}\frac{h(\cos^{-1}x)}{\sqrt{1-x^2}}dx \approx \frac{\pi}{n}\sum_{i=1}^{n} h\left(\frac{(2i-1)\pi}{2n}\right). \tag{1.85}$$

We can, however, constructed the 'closed' Gauss-Chebyshev rule by including the endpoints $\xi_0=1$ and $\xi_n=-1$ as additional nodes. Then we get a rule with nodes $\xi_i=\cos(i\pi/n)$, $i=0,1\cdots,n$, and weights $w_i=\pi/n$ for $i=1,2,\cdots,N$, and $w_0=w_n=\pi/(2n)$. Thus, the '*closed*' Gauss-Chebyshev rule is

$$\int_{-1}^{1}\frac{h(x)}{\sqrt{1-x^2}}dx \approx \frac{\pi}{n}\sum_{j=0}^{n}{}'' h\left(\cos\frac{i\pi}{n}\right). \tag{1.86}$$

This rule can be obtained from the repeated trapezoidal rule by the same method as used in showing the relationship of the open Gauss-Chebyshev rule to the midpoint rule, although the relation does not clarify why the rule is of high degree. In practice we do not generally use the closed rule because sometimes it is not possible to include the endpoint nodes. However, the closed rule has the advantage in a situation where closed rule the n points ξ_i are the subject of the $2n$ points ξ_i, and the previous function evaluations can be used again.

There are two Gauss-Chebyshev Rules on an arbitrary interval $[c_1,c_2]$:

1. Using the Gauss-Chebyshev polynomials of the first kind, $T_n(x)$, where $T_n(1)=1/2^{n-1}$, we have

$$\int_{c_1}^{c_2} \frac{h(y)}{\sqrt{(y-c_1)(c_2-y)}}dy = \frac{c_2-c_1}{2}\sum_{i=1}^{n} w_i h(y_i)+R_n, \tag{1.87}$$

where the nodes $y_i = \frac{c_2+c_1}{2} + \frac{c_2-c_1}{2}x_i$, with $x_i = \cos\frac{(2i-1)\pi}{2n}$; the weights are the same as above.

2. Using the Chebyshev polynomials of the second kind

$$U_n(x) = \frac{\sin[(n+1)\arccos x]}{\sin(\arccos x)}, \tag{1.88}$$

we get

$$\int_{c_1}^{c_2} h(y)\sqrt{(y-c_1)(c_2-y)}dy = \left(\frac{c_2-c_1}{2}\right)^2 \sum_{i=1}^{n} w_i h(y_i)+R_n, \tag{1.89}$$

where the nodes are y_i and the weights are the same as in 1 above.

1.7.5 Gauss-Kronrod rules

A $(2n+1)$-point Gauss-Kronrod rule by DIRK (1997) for the integral

$$Ih = \int_{c_1}^{c_2} h(x)ds(x), \tag{1.90}$$

where s is a nonnegative measure on the interval $[c_1, c_2]$, is a formula of the form

$$K^{(2m+1)}h = \sum_{i=1}^{2m+1} w_i h(x_i) \tag{1.91}$$

with the properties:

- m nodes of $K^{(2m+1)}$ coincide with those of the m-point Gaussian quadrature rule $G^{(n)}$ for the same measure;
- $K^{(2m+1)}h = Ih$ whenever h is polynomial of degree less than or equal to $3n+1$.

To approximate definite integrals of the form

$$\int_{c_1}^{c_2} h(x)dx \tag{1.92}$$

by using n-point Gaussian quadrature

$$\int_{c_1}^{c_2} h(x)dx \approx \sum_{i=1}^{n} w_i h(x_i), \tag{1.93}$$

where w_i, x_i are the weights and points at which to evaluate the function $h(x)$. If the interval $[c_1,\ c_2]$ is subdivided, the Gauss evaluation points of the new subintervals never coincide with the previous evaluation points (except at the midpoint for odd numbers of evaluation points), and thus the integrand must be evaluated at every point. Gauss Kronrod formulas are extensions of the Gauss quadrature formulas generated by adding $n+1$ points to an $n-$point rule in such a way that the resulting rule is of order $3n+1$. These extra points are the zeros of Stieltjes polynomials. This allows for computing higher-order estimates while reusing the function values of a lower-order estimate. The difference between a Gauss quadrature rule and its Kronrod extension are often used as an estimate of the approximation error.
Patterson (1968) showed how to find further extensions of this type.

In numerical mathematics, the Gauss-Kronrod quadrature formula is a method for numerical integration (calculating approximate values of integrals). Gauss Kronrod quadrature is a variant of Gaussian quadrature, in which the evaluation points are chosen so that an accurate approximation can be computed by re-using the information produced by the computation of a less accurate approximation. It is an example of what is called a nested quadrature rule: for the same set of function evaluation points, it has two quadrature rules, one higher order and one lower order (the latter called an embedded rule). The difference between these two approximations is used to estimate the calculational error of the integration.

These formulas are named after Alexander Kronrod, who invented them in the 1960s, and Carl Friedrich Gauss. Gaussian quadrature is used in the QUADPACK library, the GNU Scientific Library, the NAG Numerical Libraries and R (Hazewinkel and Michiel, 2001).

1.7.6 Other Forms of Gauss Quadrature

The integration problem can be expressed in a slightly more general way by introducing a positive weight function $\omega(x)$ into the integrand, and allowing an interval other than $[-1,1]$ say $[c_1,c_2]$. That is, the problem is to calculate

$$\int_{c_1}^{c_2} \omega(x)h(x)dx \tag{1.94}$$

for some choices of c_1, c_2, and $\omega(x)$. For $c_1 = -1$, $c_2 = 1$, and $\omega(x) = 1$, the problem is the same as that considered above (section 1.1). Other choices lead to other integration rules mentioned in the table below.

Table 1.1: Details are given in Abramowitz and Stegun (1972)

Interval	$\omega(x)$	Orthogonal polynomials	QT
$[-1,1]$	1	Legendre polynomials	GLQ
$(-1,1)$	$(1-x)^{\alpha}(1+x)^{\beta}$, $\alpha,\beta > -1$	Jacobi polynomials ($\beta = 0$)	GJQ
$(-1,1)$	$\frac{1}{\sqrt{1-x^2}}$	Chebyshev polynomials (first kind)	GChQ
$[-1,1]$	$\sqrt{1-x^2}$	Chebyshev polynomials (second kind)	GChQ
$[0,\infty)$	e^{-x}	Laguerre polynomials	GLgQ
$[0,\infty)$	$x^{\alpha}e^{-x}$, $\alpha > -1$	Generalized Laguerre polynomials	GLgQ
$(-\infty,\infty)$	e^{-x^2}	Hermite polynomials	GHQ

1.7.7 Fundamental theorem

Let p_n be a nontrivial polynomial of degree n such that

$$\int_{c_1}^{c_2} \omega(x)x^k p_n(x)dx = 0, \text{for all } k = 0,1,2,\cdots,n-1 \tag{1.95}$$

If we pick the n nodes x_i to be the zeros of p_n, then there exist n weights w_i which make the Gauss-quadrature computed integral exact for all polynomials $h(x)$ of degree $2n-1$ or less. Furthermore, all these nodes x_i will lie in the open interval (c_1, c_2) (Stoer and Bulirsch, 2002).

The polynomial p_n is said to be an orthogonal polynomial of degree n associated to the weight function $\omega(x)$. It is unique up to a constant normalization factor.

The idea underlying the proof is that, because of its sufficiently low degree, $h(x)$ can be divided by $p_n(x)$ to produce a quotient $q(x)$ of degree strictly lower than n, and a remainder $r(x)$ of still lower degree, so that both will be orthogonal to $p_n(x)$, by the defining property of $p_n(x)$. Thus

$$\int_{c_1}^{c_2} \omega(x)h(x)dx = \int_{c_1}^{c_2} \omega(x)r(x)dx \tag{1.96}$$

Because of the choice of nodes x_i, the corresponding relation

$$\sum_{i=1}^{n} \omega_i h(x_i) = \sum_{i=1}^{n} \omega_i r(x_i) \tag{1.97}$$

holds also. The exactness of the computed integral for $h(x)$ then follows from corresponding exactness for polynomials of degree only n or less (as is $r(x)$).

1.7.8 Errors of Gauss-Quadrature formula

The error of a Gaussian quadrature rule can be stated as follows (Stoer and Bulirsch, 2002). For an integrand which has $2n$ continuous derivatives,

$$\int_{c_1}^{c_2} w(x)h(x)dx - \sum_{i=1}^{n} w_i h(x_i) = \frac{h^{2n}(\zeta)}{(2n)!}\langle p_n, p_n\rangle \tag{1.98}$$

for some $\zeta \in (c_1,\ c_2)$, where p_n is the monic (i.e. the leading coefficient is 1) orthogonal polynomial of degree n and where

$$\langle h, g\rangle = \int_{c_1}^{c_2} w(x)h(x)g(x)dx \tag{1.99}$$

In the important special case of $w(x) = 1$, we have the error estimate (Kahaner et al., 1989)

$$\frac{(c_2 - c_1)^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} h^{2n}(\zeta), c_1 < \zeta < c_2 \tag{1.100}$$

In the research work of Stoer and Bulirsch (2002) remark that this error estimate is inconvenient in practice, since it may be difficult to estimate the order $2n$ derivative, and furthermore the actual error may be much less than a bound established by the derivative. Another approach is to use two Gaussian quadrature rules of different orders, and to estimate the error as the difference between the two results.

Important consequence of the above equation is that Gaussian quadrature of order n is accurate for all polynomials up to degree $2n-1$.

1.8 Summary

In this chapter we discussed on background of the research study, provided the problem statement, presented the objectives of the research work, gives the scope of the study, presented the limitations of the study, briefly gives the outline of the thesis and provided the basic concepts and definitions useful in understanding the study area of the research.

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